

(19) World Intellectual Property  
Organization  
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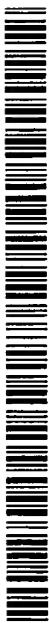


(43) International Publication Date  
5 February 2004 (05.02.2004)

PCT

(10) International Publication Number  
**WO 2004/011640 A1**

- (51) International Patent Classification<sup>7</sup>: C12N 9/48, (74) Agent: HOSODA, Yoshinori; c/o Hosoda International Patent Office, OMM Building 5th Floor, P.O. Box 26, 7-31, Otemae 1-chome, Chuo-ku, Osaka-chi, Osaka 540-6591 (JP).
- (21) International Application Number: PCT/JP2003/009523
- (22) International Filing Date: 28 July 2003 (28.07.2003)
- (25) Filing Language: English
- (26) Publication Language: English
- (30) Priority Data: 60/398,761 29 July 2002 (29.07.2002) US
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- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).
- Published:**
- with international search report
  - before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments
- For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.*



**WO 2004/011640 A1**

(54) Title: THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

(57) Abstract: A crystal of a dipeptidyl peptidase IV; a three-dimensional structural coordinate of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional coordinate of a homolog protein of the dipeptidyl peptidase IV; a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV; a method for identifying pharmacophore of the effector of the dipeptidyl peptidase IV; a method for designing, identifying, evaluating or searching; the effector; and a program and a medium therefor for use of the three-dimensional structural coordinate.

## DESCRIPTION

### THREE-DIMENSIONAL STRUCTURE OF DIPEPTIDYL PEPTIDASE IV

#### 5 TECHNICAL FIELD

The present invention relates to a crystal and a three-dimensional structural coordinate of a dipeptidyl peptidase IV, and an application thereof. More specifically, the present invention relates to a crystal and a three-dimensional structural coordinate, a method for obtaining a three-dimensional structural coordinate of a homolog protein of a dipeptidyl peptidase IV, a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV with an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, a method for identifying a pharmacophore of an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, a method for identifying sites affecting the activity of the dipeptidyl peptidase IV, a method for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, and a program and a medium therefor for use of the three-dimensional structural coordinate, which are useful in the development of an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like; and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

## BACKGROUND ART

Dipeptidyl peptidase IV (hereinafter also referred to as DPPIV) is a cell membrane protein, which has been found in epithelial cell of small intestine, prostate gland, renal tubule, biliary tract and the like, activated T-cell, B-cell, NK-cell and the like. In the DPPIV, deduced active sites of DPPIV in the C-terminal side are located in extracellular portions and those in the N-terminal side are located in cytoplasm in a living body. Also, there has been suggested the relationship of the above-mentioned DPPIV with the activities of various cytokines such as interleukin-1 $\beta$ , interleukin-2, interleukin-3, interleukin-5, interleukin-6, interleukin-13, tumor necrosis factor- $\beta$  and the like, and activities of various chemokines such as RANTES and the like in immune system [*Rinsho Menneki (Clinical Immunology)*, 34, Revised and Enlarged Edition 19, 45-53, published by Kagaku Hyoronsha (2000), and the like].

As to the dipeptidyl peptidase IV, it has been shown that some amino acid residues can be involved in exhibition of the activity of the dipeptidyl peptidase IV by experiments such as biochemical experiments using inhibitors, experiments using mutants produced by site-directed mutagenesis [for example, see Misumi et al, *Biochim. Biophys. Acta*, 1131, 333-336 (1992), Ogata et al, *Biochemistry*, 31, 2582-2587 (1992) and the like].

However, it is difficult to know the three-dimensional structures for active sites from the information. Therefore, it is presently difficult to obtain the three-dimensional structural information for identifying, searching, evaluating or designing an interaction of the dipeptidyl peptidase IV and a compound that acts with the dipeptidyl peptidase IV on the level of three-dimensional structure and a

novel compound capable of binding with and acting on the dipeptidyl peptidase IV.

#### DISCLOSURE OF INVENTION

5           A first object of the present invention is to provide a crystal of a dipeptidyl peptidase IV, which is useful for providing a three-dimensional structural coordinate as the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent  
10   for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A second object of the present invention is to provide a three-dimensional structural coordinate of the crystal, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a  
15   modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. A third object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV, whereby  
20   refinement of a three-dimensional structural coordinate of a homolog protein of the dipeptidyl peptidase IV can be more readily performed. Furthermore, a fourth object of the present invention is to provide a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which  
25   can provide the information for designing, identifying, evaluating or searching an

effector (e.g. inhibitor) of the dipeptidyl peptidase IV which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV. A fifth object of the present invention is to provide a method for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can provide the information for designing, identifying, evaluating or searching an effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body, and which can be favorably act on the dipeptidyl peptidase IV. A sixth object of the present invention is to provide a method for designing, identifying, evaluating or searching the effector (e.g. inhibitor) of the dipeptidyl peptidase IV, which can logically and conveniently provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency in a living body (*in vivo*), and which can be favorably act on the dipeptidyl peptidase IV. A seventh object of the present invention is to provide the effector (e.g. inhibitor) of the dipeptidyl peptidase IV useful as a modulatory agent of immune

response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. An eighth object of the present invention is to provide a program and a medium therefor, which can rapidly and conveniently perform design,  
5 identification, evaluation or search of the effector (e.g. inhibitor) of the dipeptidyl peptidase IV.

Concretely, the present invention relates to:

- [1] a crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the  
10 side chain level by X-ray crystallographic structural analysis;
- [2] the crystal according to the above [1], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV;
- [3] the crystal according to the above [1] or [2], wherein the dipeptidyl  
15 peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof;
- [4] the crystal according to any one of the above [1] to [3], wherein the  
20 crystal has a space group of  $P2_12_12_1$ , and a lattice constant of the unit cell of  $|a| = 118.0 \pm 5.0 \text{ \AA}$ ,  $|b| = 125.9 \pm 5.0 \text{ \AA}$ ,  $|c| = 136.8 \pm 5.0 \text{ \AA}$ , and  $\alpha = \beta = \gamma = 90^\circ$ , and is orthorhombic;
- [5] the crystal according to any one of the above [1] to [4], wherein the crystal has the structural coordinate shown in Figure 4;
- 25 [6] the crystal according to any one of the above [1] to [4], wherein the

crystal has a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;

[7] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4;

5 [8] a three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein;

[9] the three-dimensional structural coordinate according to the above [8], wherein the fluctuation of a protein is a state that is caused by molecular  
10 oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body;

[10] the three-dimensional structural coordinate according to any one of the above [7] to [9], wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl  
15 peptidase IV;

[11] the three-dimensional structural coordinate according to any one of the above [7] to [10], wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a  
20 C-terminal side or N-terminal side thereof;

[12] a three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):

(a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid  
25 sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

- 5 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

- 10 (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues located in the adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and

- 20 (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

25 all or a part of a group of amino acid residues comprising amino acids

- capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,
- 5 wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV;
- [13] the three-dimensional coordinate according to the above [12], wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK;
- 10 [14] a method for obtaining a three-dimensional coordinate of a homolog protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;
- 15 [15] a method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13], to give a three-dimensional structural coordinate;
- 20 [16] a method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or
- 25

a part of the three-dimensional structural coordinate of any one of the above [7] to [13], and the steric conformation of the effector of the dipeptidyl peptidase IV; [17] a method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of the above [7] to [13];

[18] the method according to the above [17], wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:

- (i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of the above [7] to [13] and the steric conformation of the effector of the dipeptidyl peptidase IV;
- (ii) identifying atoms or atomic groups capable of generating in the above region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
- (iii) designing a compound based on the information of the above step (i) and/or (ii);

[19] the method according to the above [18], wherein the method further comprises the steps of:

- detecting an interaction between the dipeptidyl peptidase IV and the

designed, identified, evaluated or searched candidate compound,  
wherein when an interaction is detected, the candidate compound is identified as  
a compound capable of binding to the dipeptidyl peptidase IV, based on a degree  
of the interaction as an index;

5 [20] the method according to the above [18] or [19], wherein the method  
further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified,  
evaluated or searched candidate compound and measuring the activity of the  
dipeptidyl peptidase IV,

10 wherein when an activity increases or decreases, the designed, identified,  
evaluated or searched candidate compound is identified as a compound having  
enhancing action or inhibitory action on the activity of the dipeptidyl peptidase  
IV, based on a degree of the increase or decrease as an index;

[21] an effector of the dipeptidyl peptidase IV obtainable by the method of any  
15 one of the above [17] to [20];

[22] a program and a medium therefor for use of the three-dimensional  
structural coordinate of any one of the above [7] to [13], wherein all and/or a part  
of the three-dimensional structural coordinate of any one of the above [7] to [13]  
is recorded;

20 [23] the program and the medium according to the above [22], comprising a  
means for identifying, searching, evaluating or designing a compound capable of  
binding to the dipeptidyl peptidase IV or a compound having an enhancing  
action or inhibitory action on the activity for the dipeptidyl peptidase IV; and

[24] the program and the medium according to the above [23], further  
25 comprising a means for displaying a three-dimensional graphic display of a

molecule.

#### BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 is a photomicrograph of a crystal of a dipeptidyl peptidase IV,  
5 wherein the field of view is  $4000\ \mu\text{m} \times 3000\ \mu\text{m}$ .

Figure 2 is a photograph for X-ray diffraction pattern of a crystal of dipeptidyl peptidase IV.

Figure 3 is a photograph showing a three-dimensional structure of a crystal of a dipeptidyl peptidase IV displayed by the program QUANTA  
10 (Accelrys, Inc.).

Figure 4 is a drawing showing a three-dimensional coordinate of a crystal of a dipeptidyl peptidase IV.

#### BEST MODE FOR CARRYING OUT THE INVENTION

15 In the present specification, amino acid residues are expressed by using the following abbreviations, which have been adopted by the IUPAC-IUB Commission on Biochemical Nomenclature (CBN). Also, unless explicitly otherwise indicated, the amino acid sequences of peptides and proteins are identified from N-terminal to C-terminal, left terminal to right terminal, the  
20 N-terminal being identified as a first residue. Ala: alanine residue; Asp: aspartate residue; Glu: glutamate residue; Phe: phenylalanine residue; Gly: glycine residue; His: histidine residue; Ile: isoleucine residue; Lys: lysine residue; Leu: leucine residue; Met: methionine residue; Asn: asparagine residue; Pro: proline residue; Gln: glutamine residue; Arg: arginine residue; Ser: serine  
25 residue; Thr: threonine residue; Val: valine residue; Trp: tryptophane residue;

Tyr: tyrosine residue; Cys: cysteine residue.

The crystal of the present invention is a crystal of a dipeptidyl peptidase IV, having a characteristic sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray  
5 crystallographic structural analysis.

The “characteristic sufficient to ensure a resolution capable of analyzing three-dimensional structure up to the side chain level” is, for example,  
(1) being in a state that a molecule in a unit cell of a crystal has repeats with high regularity, namely, providing diffraction at high resolution;  
10 (2) having suitable form and size; it is desired that for example, a crystal has at least one side grown to about 0.2 to about 0.5 mm, preferably a cubic crystal having three sides that have similarly grown, or a needle-shaped crystal having a width or thickness of about 0.2 mm or more;  
(3) having chemical stability, dynamic stability and physical stability;  
15 and the like. In a case of the dipeptidyl peptidase IV, which is a polypeptide having a relatively large molecular weight, the term means characteristics sufficient to ensure a resolution of 3Å or less, preferably 2.8Å or less, more preferably 2.6Å or less.

The dipeptidyl peptidase IV used for the preparation of the crystal of the  
20 present invention may have a high purity sufficient for forming the crystal. In the present invention, the dipeptidyl peptidase IV used for the preparation of the crystal includes a soluble polypeptide consisting of a region located at extramembrane in a full-length human dipeptidyl peptidase IV, for example, a polypeptide in which a transmembrane region in the N-terminal side [namely the  
25 region including the transmembrane sites (the region containing at least the

amino acid nos: 1-28 of SEQ ID NO: 2, preferably the region of the amino acid  
nos: 1-32)] is deleted from the amino acid sequence of a full-length human  
dipeptidyl peptidase IV of SEQ ID NO: 2, and a tag peptide is optionally added  
to a C-terminal side or N-terminal side of the amino acid sequence. Concrete  
5 examples include (I) a polypeptide in which a transmembrane region in the  
N-terminal side is deleted from the amino acid sequence of a full-length human  
dipeptidyl peptidase IV of SEQ ID NO: 2; and (II) a polypeptide in which a tag  
peptide is added to a C-terminal side or N-terminal side of the polypeptide of the  
above (I). In the polypeptide, since the transmembrane site is deleted therefrom,  
10 the polypeptide has excellent characteristics that anchoring to the membrane can  
be prevented, and the polypeptide is a secretory type and soluble. The tag  
peptide is not particularly limited. For example, a polyhistidine peptide (an  
oligopeptide consisting of 4 to 20 of histidine residues) or the like can be  
preferably used as the tag peptide.

15 SEQ ID NO: 2 shows the amino acid sequence of a full-length dipeptidyl  
peptidase IV of human colon.

The full-length dipeptidyl peptidase IV means a polypeptide of a  
dipeptidyl peptidase IV containing a region comprising a transmembrane site in  
the N-terminal side. The full-length dipeptidyl peptidase IV includes a  
20 polypeptide comprising the amino acid sequence of SEQ ID NO: 2, without  
being limited thereto, and encompasses its naturally occurring variant, artificially  
modified variant, a homolog and an ortholog derived from heterogeneous  
organism, and the like.

Concretely, the full-length dipeptidyl peptidase IV, besides the  
25 polypeptide comprising the amino acid sequence of SEQ ID NO: 2, includes

conservative substitution variants, naturally occurring allelic variants and the like. Also, the full-length dipeptidyl peptidase IV includes a polypeptide having at least one, namely one or more conservative amino acid substitutions, as compared to the polypeptide comprising the amino acid sequence of  
5 SEQ ID NO: 2.

The polypeptide as described above may be a polypeptide having biological activities (namely dipeptidyl peptidase IV activity) similar to the polypeptide comprising the amino acid sequence of SEQ ID NO: 2. Concretely, there are included, for instance, a polypeptide having homology of usually about  
10 80% or more, preferably about 90% or more, more preferably about 95% or more on the amino acid level, as compared to the full-length amino acid sequence of SEQ ID NO: 2; a polypeptide encoded by a nucleic acid capable of hybridizing with a nucleic acid consisting of the nucleotide sequence of SEQ ID NO: 1 (nucleotide sequence encoding a full-length dipeptidyl peptidase  
15 IV of human colon), under stringent conditions, or a complement thereof; and a polypeptide having deletion, substitution or addition of at least one amino acid, namely one or plural amino acids, preferably one or several amino acids in the amino acid sequence of SEQ ID NO: 2.

The number of deletion, substitution or addition of the amino acids may  
20 be to an extent that the biological activities [namely, dipeptidyl peptidase IV activity] are not lost, usually in the number of 1 to about 150, preferably 1 to about 75, more preferably 1 to about 40.

The crystallization is carried out by making a solution containing the desired protein (referred to as a protein solution) supersaturated state, based on  
25 the characteristics that the protein in solution state converts to non-soluble state

and precipitates as a crystal when specific conditions are satisfied. Concretely, the protein can be precipitated by the following procedures 1. or 2.:

1. elevating the effective concentration of the protein:

concretely, adding a precipitant such as a salt, polyethylene glycol or an organic solvent to a protein solution; reducing an amount of a solvent in the protein solution by evaporation or the like; or the like.

2. reducing a repulsive force, or increasing an attractive force between protein molecules:

concretely, adding an organic solvent such as an alcohol to a protein solution; changing a hydrogen ion concentration (pH) or temperature of the protein solution; or the like.

As the conditions for the crystallization, physical and chemical factors such as a hydrogen ion concentration (pH), a kind of buffer used and a concentration thereof, a kind of a precipitant added and a concentration thereof, protein concentration, salt concentration, temperature and the like can be involved. A method for controlling and investigating the factors includes batch methods, dialysis methods, vapor diffusion methods (hanging-drop method, sitting-drop method and the like) and the like, described, for instance, in Blundell, T. L. et al., *PROTEIN CRYSTALLOGRAPHY*, 59-82 (1976), published by Academic Press, or the like.

The method for crystallization includes the batch methods, dialysis methods, vapor diffusion methods and the like. By the above method, physical and chemical factors such as a hydrogen ion concentration (pH), a kind and a concentration of the buffer used, and a kind and a concentration of the precipitant used, and physical and chemical factors such as protein concentration, salt

concentration and temperature can be also determined.

The hydrogen ion concentration (pH) can be adjusted with a buffer. It is desired that the buffer is a buffer having buffering action in a broad range of pH, and being capable of suppressing precipitation of a non-proteinous crystal  
5 between the co-existing ion in the solution used during crystallization and the precipitant or the like. The buffer includes Tris-hydrochloric acid buffer, phosphate buffer, cacodylate buffer, acetate buffer, citrate buffer, glycine buffer and the like.

The precipitant may be a substance capable of elevating an effective  
10 concentration of the protein or changing a hydrogen ion concentration (pH) of the protein solution. Generally, the precipitant includes salts such as ammonium sulfate, sodium sulfate, sodium phosphate, potassium phosphate, sodium citrate, ammonium citrate, sodium chloride, potassium chloride and ammonium chloride; polyethylene glycols having various average molecular weights of  
15 about 200, about 1000, about 2000, about 4000, about 6000, about 8000, about 20000 or the like; organic solvents such as 2-methyl-2,4-pentadiol, methanol, ethanol, isopropanol, butanol and acetone, and the like.

The protein concentration may be a concentration suitable for crystallization, and it is desired that the protein concentration is, for example, 1  
20 to 50 mg/ml, preferably 5 to 20 mg/ml, more preferably 7 to 15 mg/ml.

It is desired that the temperature conditions are 3° to 25°C, preferably 12° to 22°C.

In the case where the crystallization is carried out by the batch method, the crystallization can be carried out by gradually adding a precipitant solution  
25 comprising a precipitant, buffer and the like, so as to form a layer on the top

layer of the solution containing the dipeptidyl peptidase IV to give a mixture, or by gradually adding the solution comprising the dipeptidyl peptidase IV, so that the solution is an upper layer of the precipitant solution to give a mixture. Here, the mixture is allowed to stand in a tightly closed vessel.

5           In the case where the crystallization is carried out by the dialysis method, the crystallization can be carried out by placing a solution comprising dipeptidyl peptidase IV in a size exclusion semi-permeable membrane, and placing a precipitant solution outside of the size exclusion semi-permeable membrane as a reservoir solution, thereby diffusing the reservoir solution to the solution  
10           comprising the dipeptidyl peptidase IV via the semi-permeable membrane.

          In the case where the crystallization is carried out by the hanging-drop method in the vapor diffusion method, the crystallization can be carried out by placing a mixed solution of a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel allowing to be hanged at a position  
15           above the upper space of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

          In the case where the crystallization is carried out by the sitting-drop method in the vapor diffusion method, the crystallization can be carried out by  
20           placing a mixed solution comprising a solution comprising the dipeptidyl peptidase IV and a precipitant solution in a closed vessel at a position higher than the liquid surface of a reservoir in which the precipitant solution is contained as a reservoir solution, wherein the vapor pressure of the reservoir solution in the reservoir is set to be lower than that of the mixed solution.

25           The crystallization can be carried out by the sitting-drop method from the

viewpoint of obtaining excellent-quality and large crystal.

When the obtained crystal is a crystal insufficient to ensure the X-ray structural analysis, the crystal may be grown by a seeding method such as macro-seeding method or micro-seeding method, using the obtained crystal as a seed crystal.

When the macro-seeding method is performed, it is desired that the seed crystal is a single crystal that can be isolated by procedures under microscope wherein the seed crystal has excellent external form (having excellent crystallinity). Also, it is desired that the seed crystal is washed with a drop of a solution obtained by diluting the precipitant, for example, by 0.5 to 1.0-fold. It is desired that the solution used for seeding of the seed crystal is a protein solution having a degree of supersaturation that the crystal grows but the crystal nuclei do not grow. On the other hand, when the micro-seeding method is performed, the form and size of the seed crystal are not particularly limited.

The sequence information for the dipeptidyl peptidase IV and cDNA encoding the dipeptidyl peptidase IV can be obtained from a known information source [GenBank/EMBL accession No: X60708; Misumi et al., *Biochim. Biophys. Acta*, **1131**, 333-336, (1992); GenBank/EMBL accession No: M80536; Darmoul et al., *J. Biol. Chem.*, **267**, 4824-4833, (1992)]. Therefore, the dipeptidyl peptidase IV or a soluble polypeptide thereof can be produced by using conventional means for gene engineering on the basis of the above sequence information.

The nucleic acid used for production of the dipeptidyl peptidase IV or a soluble polypeptide thereof may be any nucleic acid in which the encoded polypeptide exhibits a dipeptidyl peptidase IV activity. For example, a nucleic

acid encoding a polypeptide consisting of the amino acid sequence in which a transmembrane region in the N-terminal side (a region containing at least the amino acid nos: 1-28, preferably the region of the amino acid nos: 1-32) is deleted from the full-length human dipeptidyl peptidase IV, and a tag peptide is  
5 optionally added to a C-terminal side or N-terminal side of the amino acid sequence.

The nucleic acid can be obtained by, for instance, obtaining a fragment comprising a nucleic acid encoding a full-length dipeptidyl peptidase IV or a part thereof by means of conventional DNA recombination technique, and  
10 appropriately arranging the obtained fragment.

SEQ ID NO: 1 shows a sequence of a nucleic acid encoding a full-length dipeptidyl peptidase IV of human colon.

The nucleic acid (DNA or RNA) encoding a full-length dipeptidyl peptidase IV includes, for instance, a nucleic acid comprising human nucleic  
15 acids comprising the nucleotide sequence of SEQ ID NO: 1 without being limited thereto, and includes its naturally occurring variant, artificially modified variant, a homolog or ortholog derived from heterogeneous organism.

In other words, besides the nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1, the nucleic acid includes a nucleic acid capable of  
20 hybridizing with a nucleic acid comprising the nucleotide sequence of SEQ ID NO: 1 under stringent conditions, more preferably under high-stringent conditions), or a complement thereof (nucleic acid having a complementary sequence).

Concrete examples of the nucleic acid described above include, for  
25 instance, a nucleic acid having usually about 70% or more, preferably about 80%

or more, more preferably about 85% or more, still more preferably about 90% or more, still more preferably about 95% or more, homology to the nucleotide sequence of SEQ ID NO: 1, and it is preferable that the polypeptide encoded by the above nucleic acid has a dipeptidyl peptidase IV activity.

5           The dipeptidyl peptidase IV activity can be measured by, for example, incubating in a 1.5 ml reaction mixture [composition: 1.5 mM substrate (Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes, and determining the liberated paranitroanilide at the absorbance of 405 nm. One unit (1 U) of a dipeptidyl peptidase IV is defined as an amount of  
10           the enzyme required for liberating 1  $\mu$ mol of paranitroanilide per 1 minute.

          In the present invention, the hybridization under stringent conditions can be carried out as normal stringent conditions by performing hybridization in a hybridization solution having a salt concentration of  $6 \times$  SSC or an equivalent concentration thereto, under the temperature conditions of 50° to 70°C for about  
15           16 hours, and optionally performing pre-washing with a solution having a salt concentration of  $6 \times$  SSC or an equivalent concentration thereto, and thereafter performing washing with a solution having a salt concentration of  $1 \times$  SSC or an equivalent concentration thereof. Furthermore, as the conditions having still higher stringency (high-stringent conditions), the hybridization can be carried out  
20           by washing with a solution having a salt concentration of  $0.1 \times$  SSC or an equivalent concentration thereto in the above method.

          The dipeptidyl peptidase IV used for the crystallization has purity that can form a crystal, and the purity can be confirmed by conventional means of confirming purity (for example, a method comprising electrophoresing a fraction  
25           by polyacrylamide gel electrophoresis, SDS-polyacrylamide gel electrophoresis

or the like, and visualizing the fraction by silver staining, or the like).

The X-ray structural analysis data of the crystal can be obtained by subjecting the crystal of the present invention to an X-ray crystallographic structural analysis known to one of ordinary skill in the art [for example, see  
5 Blundell, T. L. et al., *PROTEIN CRYSTALLOGRAPHY*, 59-82 (1976), published by Academic Press, and the like], whereby a three-dimensional structural coordinate (a value showing the relationship of the spatial positions of each atom) and a three-dimensional structure model for the crystal can be obtained. Concretely, the three-dimensional structural coordinate of the dipeptidyl  
10 peptidase IV is obtained as an atomic coordinate by procedures comprising the steps of 1) irradiating the crystal of the present invention with a monochromatic X-ray to give an X-ray diffraction pattern, 2) obtaining X-ray diffraction intensity data from the X-ray diffraction pattern, 3) obtaining an electron density map by Fourier transform, and 4) allocating a polypeptide chain and side chain  
15 thereof on the electron density map based on the amino acid sequence of the polypeptide used for the crystal. Furthermore, the three-dimensional structure is clarified by molecule-modeling based on the three-dimensional structural coordinate. Therefore, the three-dimensional structural coordinate of the dipeptidyl peptidase IV obtained from the crystal of the present invention is also  
20 encompassed within the scope of the present invention.

The crystallographic parameters for the crystal are obtained from the X-ray diffraction intensity data of the crystal of the present invention. The crystal of the present invention is an orthorhombic crystal having a space group of  $P2_12_12_1$ , and a lattice constant of the unit cell of  $|a| = 118.0 \pm 5.0 \text{ \AA}$ ,  
25  $|b| = 125.9 \pm 5.0 \text{ \AA}$ ,  $|c| = 136.8 \pm 5.0 \text{ \AA}$ , and  $\alpha = \beta = \gamma = 90^\circ$ . The crystal has a

2.6Å resolution by X-ray crystallographic structural analysis, that is, the crystal has characteristics sufficient to ensure a resolution capable of analyzing up to the side chain level of the polypeptide.

5 It is a known fact to one of ordinary skill in the art that the same protein can be crystallized even under different conditions. Therefore, the present invention is not limited to only the conditions for crystallization, and the crystal that shows substantially the same crystallographic constants as those in the present invention are also encompassed within the scope of the present invention.

10 More concretely, the crystal of the dipeptidyl peptidase IV of the present invention has a structural coordinate as shown in Figure 4, or a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

15 The crystal according to the present invention can also be used as a seed crystal for carrying out the crystallization of a polypeptide having a three-dimensional structure similar to that of the dipeptidyl peptidase IV used for, for example, carrying out the crystallization of the dipeptidyl peptidase IV, dipeptidyl peptidase IV-like proteins, homolog proteins and the like, which are derived from other organism species.

20 When the crystal of the present invention is irradiated with X-ray, a low-temperature measurement may be carried out, as described in Examples set forth below.

25 The X-ray structural analysis data are converted to a structure factor by evaluating the intensity of X-ray diffraction using MOSFILM Program Package (Version 6.1). Also, in order to obtain the information for the phase, multiple isomorphous replacement method or the like can be performed, for example, as

described in Examples.

In the structural analysis, CCP4 (Collaborative Computational Project, Number 4, 1994, "*The CCP4 Suite: Programs for Protein Crystallography*," *Acta Cryst.* D50, 760-763) program or the like is used.

5           The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be obtained, for example, as follows. Firstly, Fourier transform calculation is carried out using the differences between the diffraction intensity obtained from two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from native crystal, and  
10   investigating the large peaks provided by the heavy atoms (mercury) on the Patterson's diagram to determine the locations of each mercury atoms in the unit cell of the real space. The phase of the crystal structure factor for the native crystal is determined using the obtained location coordinate for the mercury atoms. Furthermore, refinement is performed using the crystal structure factor of  
15   the native crystal and two kinds of the crystal structure factors of the isomorphous replacement crystals of mercury, and the coordinate for each of the mercury atoms is more accurately determined. An electron density map for the crystal of the dipeptidyl peptidase IV in the real space is obtained using the phase of the crystal structure factor of the native crystal calculated from the refined  
20   mercury atoms coordinate. Furthermore, the electron density map is improved by performing smoothing and histogram matching for the electron density map of the solvent region, whereby an electron density map necessary and sufficient for building a molecular model can be obtained. Next, the sites corresponding to the amino acid residues of the dipeptidyl peptidase IV on the electron density  
25   map are identified using QUANTA (manufactured by Accelrys, Inc.) to build the

molecular model to give a three-dimensional structural coordinate.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is shown in Figure 4. Figure 4 shows the obtained three-dimensional structural coordinates, according to the format of the Protein Data Bank, which is a notation generally used by one of ordinary skill in the art.

The three-dimensional structural coordinates shown in Figure 4 are those represented using the origin of the unit cell of the crystal as the origin of the three-dimensional space. The R factor that is considered as an index for the accuracy of the obtained molecular model is 24.89%, and the free R factor is 30.15%. In addition, the deviation in the interatomic bond distance from the ideal state of the three-dimensional structure (rms-deviation) and the deviation in the bond angle are 0.006Å and 1.305°, respectively. In the case, for instance, the three-dimensional structural coordinate of the present invention is used for the calculation by a computer, a novel structural coordinate obtained as a result of the operation for mathematical transfer, such as translation, rotation, or symmetry in the three-dimensional space without changing the relative configuration of the atoms, is also encompassed within the scope of the present invention. Furthermore, not only all of the three-dimensional structural coordinate of the present invention but also a part thereof are also encompassed within the scope of the present invention.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be used, for example, as shown in Figure 3, for three-dimensional graphic displaying of the stereogram of the three-dimensional structure model, and for evaluation of the structure-activity relationship and the quantitative structure-activity relationship. Also, the structural features of the

crystal of the present invention can be more concretely shown using the three-dimensional structural coordinate shown in Figure 4. The evaluation of the structure-activity relationship or quantitative structure-activity relationship by the three-dimensional structure model is also encompassed within the scope of the present invention.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the dipeptidyl peptidase IV can be found in that the dipeptidyl peptidase IV has 273 molecules of bond water in an asymmetric unit and has 5 molecules of N-acetylglucosamine residues per 1 molecule of the dipeptidyl peptidase IV.

According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, interacting with the atoms or atomic groups of a known effector of the dipeptidyl peptidase IV via an intermolecular interaction can be obtained.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of regions in the dipeptidyl peptidase IV that are susceptible to binding or intermolecular interaction with the effector can be obtained.

In addition, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information of the structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be obtained. Therefore, higher selectivity in the effector targeting a protein other than the dipeptidyl peptidase IV can be designed, when the effector also acts on the dipeptidyl peptidase IV.

The intermolecular interaction includes covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like.

5 In the present specification, the atoms or atomic groups of the effector and atoms or atomic groups of the side chain of the dipeptidyl peptidase IV, which interact with each other via intermolecular interaction, are referred to as “pharmacophore.”

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the information for the structure  
10 specific for the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV, can be provided.

In addition, for example, when the measurement conditions are different in X-ray diffraction, or the three-dimensional structure of the complex in the solution is analyzed using multidimensional NMR, and the like, the three-  
15 dimensional structural coordinate may differ from that shown in Figure 4. The three-dimensional structural coordinate varies depending on the fluctuation of protein and the like, and is encompassed within the scope of the present invention.

In the present specification, the “fluctuation of protein” means a state that  
20 is caused by molecular oscillation, temperature and the like, and accompanied with the structural change that can exhibit an activity for the dipeptidyl peptidase IV in a living body.

Also, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, one of the characteristics of the  
25 dipeptidyl peptidase IV resides in that the amino acid residues, Ser 630, Asp 708

and His 740, which are involved in the activity deduced by experiments by using various active inhibitors of the dipeptidyl peptidase IV, exist in the adjacent area, even though the amino acid residues exist in distant locations on the primary sequence. Concretely, the distance between the O<sub>δ2</sub> atom of Asp 708 and the N<sub>δ1</sub> atom of His 740, and the distance between the N<sub>ε2</sub> atom of His 740 and the O<sub>γ</sub> atom of Ser 630 are distances that can form hydrogen bonding.

Therefore, the present invention also includes a three-dimensional structural coordinate of the region in the dipeptidyl peptidase IV, which is involved in binding or interaction of the dipeptidyl peptidase IV with an effector thereof, including a three-dimensional structural coordinate of a region selected from the group consisting of the following (a) to (d):

- (a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and  
all or a part of a group of amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;
- (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and  
all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids of the group of amino acid residues located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

- (c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and
- 5 all or a part of a group of amino acid residues located in the adjacent area of said group of the amino acid residue in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate; and
- (d) a region characterized by a group of amino acid residues comprising
- 10 amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and
- all or a part of a group of amino acid residues of a group of amino acid residues comprising amino acids capable of maintaining physicochemical
- 15 characteristics physiologically equivalent to the each amino acid of the amino acid residues located in the adjacent area of said groups of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate.

In the present specification, the "adjacent (area)" refers to an area

20 involved in covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction or the like with the amino acid residues, concretely, a region within 10Å, preferably within 8Å, more preferably within 5Å.

The physicochemical characteristic includes features in shape of the three-

25 dimensional structure, hydrophobicity, electric charge, pK and the like.

The "amino acid capable of maintaining physicochemical characteristics physiologically equivalent" may be an amino acid analogue residue obtained by replacing a side chain of amino acid residues in the three-dimensional structural coordinate shown in Figure 4 with other side chain, for example, showing  
5 bioisosterism. Alternatively, the amino acid residue in the three-dimensional structural coordinate shown in Figure 4, may be replaced with another amino acid residue belonging to the same Group, in any of the following Groups I to VI:

- I glycine, alanine;
- 10 II valine, isoleucine, leucine;
- III aspartic acid, glutamic acid, asparagine, glutamine;
- IV serine, threonine;
- V lysine, arginine;
- VI phenylalanine, tyrosine.

15 According to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, a three-dimensional structural coordinate of a polypeptide can be easily derived if an accurate amino acid sequence is determined, even when the polypeptide is a dipeptidyl peptidase IV or a dipeptidyl peptidase IV-like protein derived from other organism species, as long  
20 as the polypeptide is a polypeptide having high homology on the level of amino acid sequence with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention (for example, at least 20%, preferably 30% or more, more preferably 40% or more).

Furthermore, the three-dimensional structural coordinate of the dipeptidyl  
25 peptidase IV of the present invention can be used for X-ray crystallographic

structural analysis of the crystal and the like of other proteins having an amino acid sequence with significant homology with the dipeptidyl peptidase IV used for the preparation of the crystal of the present invention. Concretely, according to the molecular replacement method [for example, see Blundell, T. L. et al.,  
5 *PROTEIN CRYSTALLOGRAPHY*, 446-464 (1976), published by Academic Press and the like], the three-dimensional structural coordinate thereof can be quickly and readily obtained from the structure factors obtained by the X-ray diffraction pattern of the crystal, without using multiple isomorphous replacement method, even for the determination of the structural coordinate of the above-mentioned  
10 crystal of which structural coordinate has not yet been known.

In the present specification, the term "significant homology" is a case where there is identity of 20%, or more, preferably by 30% or more, between the amino acid sequences.

When the molecular replacement method is performed, for example, a  
15 program such as X-PLOR and CNX (both manufactured by Accelrys Inc.) or AMORE [one of the programs of CCP4 (Collaborative Computational Project, Number 4), *Acta Crystallogr. D*50, 670-673 (1994)] can be run by a computer on which the program can be executed. Here, whether or not the molecular replacement method is applicable can be determined by actually applying the  
20 molecular replacement method to the structure factors calculated from the X-ray diffraction pattern of the desired crystal and obtaining a significant solution.

In other words, the three-dimensional structural coordinate obtained by structural analysis by molecular replacement method is encompassed within the scope of the present invention as long as a significant solution is obtained. The  
25 present invention also encompasses a three-dimensional structural coordinate of

a dipeptidyl peptidase IV, or a dipeptidyl peptidase IV-like protein, namely a homolog protein or the like of other organism species derived by the above method.

Therefore, according to the present invention, a method for obtaining a  
5 three-dimensional structural coordinate of a homolog protein of a dipeptidyl  
peptidase IV comprising the step of performing refinement of an electron density  
map of the homolog protein of the dipeptidyl peptidase IV comprising the amino  
acid sequence of SEQ ID NO: 2, based on the three-dimensional structural  
coordinate of the present invention, to give a three-dimensional structural  
10 coordinate is provided. Also, a method for obtaining a three-dimensional  
structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and  
an effector of the dipeptidyl peptidase IV, based on the three-dimensional  
structural coordinate of the present invention, is likewise provided.

According to the three-dimensional structural coordinate of the dipeptidyl  
15 peptidase IV of the present invention, a method for identifying a region or site  
for a target for binding or interaction between the dipeptidyl peptidase IV and an  
effector of the dipeptidyl peptidase IV is provided, based on the analysis of the  
binding regions between the dipeptidyl peptidase IV and a known effector of the  
dipeptidyl peptidase IV such as an inhibitor, or based on the simulation of the  
20 interaction between the dipeptidyl peptidase IV and a known effector of the  
dipeptidyl peptidase IV.

Also, based on the three-dimensional structural coordinate of the  
dipeptidyl peptidase IV of the present invention and the steric conformation of  
the effector of the dipeptidyl peptidase IV, the pharmacophore of the effector of  
25 the dipeptidyl peptidase IV can be identified. A method for identifying the

pharmacophore is also provided. The method is useful for designing an effector having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency to a living body, and lower toxicity.

5           Concretely, for example, the region or site for a target involved in binding or interaction of the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV, can be identified by:

- 1)     obtaining a crystal of a complex of the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV such as an inhibitor, and obtaining  
10     a three-dimensional structural coordinate of the crystal based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV, whereby obtaining the three-dimensional structural coordinate of a binding region of the dipeptidyl peptidase IV and the effector;
- 15     2)     simulating an intermolecular interaction between the dipeptidyl peptidase IV and a known effector of the dipeptidyl peptidase IV based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;  
20     or the like.

The crystal of the above-mentioned complex can be obtained by, for example, incubating the crystal of the present invention in a solution comprising the effector, forming a complex of the dipeptidyl peptidase IV and the effector, and crystallizing the obtained complex, and the like.

25           Also, when the three-dimensional structural coordinate of the crystal of

the complex is obtained, the steric structure of the effector of the above-mentioned complex can be readily obtained by calculating the differential Fourier diagram utilizing a three-dimensional structure model defined by the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, whereby specific interaction forms and interaction sites  
5 between the dipeptidyl peptidase IV and the effector can be readily clarified.

When the intermolecular interaction is simulated, for example, the space regions, residues and the like in which covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals  
10 force, electrostatic interaction, hydrophobic interaction or the like can be simulated, based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV.

Furthermore, according to the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, the three-dimensional  
15 structural coordinate or the three-dimensional structure model based on the three-dimensional structural coordinate regarded as an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and regions or sites involved in binding or interaction with the effector, or the like, is obtained,  
20 whereby a compound capable of specifically acting on the dipeptidyl peptidase IV can be designed, identified, evaluated or searched.

For example, in the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate, a compound capable of modifying the activity of the dipeptidyl peptidase IV can be designed,  
25 identified, evaluated or searched, based on the regions characterized by Ser 630,

Asp 708 and His 740, and all or a part of amino acid residues of the group of the amino acid residues located in the adjacent area of the Ser 630, Asp 708 and His 740.

Therefore, according to the present invention, a method for designing,  
5 identifying, evaluating or searching an effector of the dipeptidyl peptidase IV is provided.

One of the significant features of the method of the present invention for designing, identifying, evaluating or searching an effector resides in that the method comprises designing, identifying, evaluating or searching a compound  
10 capable of acting on the dipeptidyl peptidase IV, based on the three-dimensional structural coordinate of the present invention.

According to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the  
15 present invention, the information for a structure specific to the dipeptidyl peptidase IV, which is not found in proteins other than the dipeptidyl peptidase IV can be obtained. Therefore, according to the method of the present invention for designing, identifying, evaluating or searching an effector, the method has an excellent effect that the selectivity of the effector of the dipeptidyl peptidase IV  
20 can be enhanced.

Also, according to the method of the present invention for designing, identifying, evaluating or searching an effector, since the method is based on the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention, visual studies and/or energy calculation can be made  
25 according to the method by using a computer and the like. Therefore, there are

exhibited some excellent effects that a compound having excellent characteristics such as having higher avidity, higher biological activity, higher biological stability, higher thermodynamic stability, higher absorbency in a living body, and lower toxicity, than those for a known inhibitor can be designed, identified,  
5 evaluated or searched, and that logical design can be performed in the three-dimensional space.

In the present specification, the "effector" includes a compound that inhibits or enhances the activity (i.e. inhibitor or activator), which may be natural compounds or synthetic compounds, or may be polymers or low-molecular  
10 weight compounds.

A concrete example of the method of the present invention for designing, identifying, evaluating or searching an effector includes a method comprising the steps of:

- (i) identifying a region to be targeted for binding or interaction with the  
15 effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of the present invention and the steric conformation of the effector of the dipeptidyl peptidase IV;
- (ii) identifying corresponding atoms or atomic groups capable of generating in the region at least one intermolecular interaction selected from the  
20 group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and
- (iii) designing a compound based on the above information of the above step  
25 (i) and/or (ii).

The three-dimensional structural coordinate used for designing, identifying, evaluating or searching a compound capable of binding to the dipeptidyl peptidase IV may be a coordinate fixed in the three-dimensional space, and the intensity of binding with the compound or the like can be calculated by carrying out translation or rotation in the three-dimensional space, and transfer to an extent that the chemical covalent bond would not be cleaved in the amino acid residues of the dipeptidyl peptidase IV.

In the above step (i), the "region to be targeted in the dipeptidyl peptidase IV" preferably includes an active center of the dipeptidyl peptidase IV, sites indirectly acting on the active center and the like. For example, there is included a region characterized by Ser 630, Asp 708 and His 740 and all or a part of a group of the amino acid residues located in the adjacent area of Ser 630, Asp 708 and His 740, and the like in the structural coordinate of Figure 4 and the three-dimensional structure model defined by the structural coordinate. The atoms or atomic groups that can be matched therewith are identified, based on the three-dimensional structural coordinate of an active center, sites indirectly acting on the active center and the like, whereby the candidate atoms or candidate atomic groups can be obtained.

In the above step (ii), for example, the atoms or atomic groups capable of associating via intermolecular interaction between the atoms or atomic groups in the region, concretely, the corresponding atoms or atomic groups capable of generating covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction, hydrophobic interaction and the like, are searched and extracted, based on the information identified in the above step (i).

Next, in the above step (iii), the corresponding atoms or atomic groups searched in the above step (i) and/or (ii) are combined to design a compound.

Thereafter, if desired, whether or not the compound designed in the above step (iii) is matched via intermolecular interaction with the side chains and atoms  
5 or atomic groups in the dipeptidyl peptidase IV as defined by the three-dimensional structural coordinate of the present invention can be simulated.

The compound designed, identified, evaluated or searched by the above steps (hereinafter also referred to as a candidate compound in the present specification) can be obtained by generally used chemical synthetic methods,  
10 depending on the compound.

In addition, in the method of the present invention for designing, identifying, evaluating or searching an effector, there can be carried out a step of detecting the interaction between the dipeptidyl peptidase IV and the candidate compound. When the interaction is detected, the interaction serves as an index  
15 showing that the above candidate compound is a compound capable of binding to the dipeptidyl peptidase IV.

The above interaction can be detected by, for example, plasmon resonance analysis apparatus, mass spectrometer, titration isothermal calorimetry, NMR and the like. For example, in the case of plasmon resonance analysis apparatus,  
20 when a sensorgram indicates the formation of a complex, by contacting the dipeptidyl peptidase IV-immobilized matrix with the candidate compound and performing analysis by optical detection (for example, photometer, polarization photometer and the like) and the like, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is  
25 generated. For example, in the case of a mass spectrometer, when a spectrum

indicates the formation of a complex, by contacting the dipeptidyl peptidase IV-immobilized matrix with the candidate compound and performing analysis with a mass spectrometer (matrix-assisted laser desorption/ionization-time of flight mass spectrometry: MALDI-TOF MS, electro spray-ionization mass spectrometer: ESI-MS and the like), it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated. For example, in the case of titration-thermal calorimetry interaction analysis, when the titration curve indicates the formation of a complex, by contacting a solution of the dipeptidyl peptidase IV with the candidate compound, and measuring the heat coming in and out of a thermal diode and the like, it would be an index showing that the interaction between the candidate compound and dipeptidyl peptidase IV is generated. For example, in the case of NMR, when a spectrum indicates the formation of a complex, by analyzing by NMR a solution prepared mixing the dipeptidyl peptidase IV and a candidate compound, it would be an index showing that the interaction between the candidate compound and the dipeptidyl peptidase IV is generated.

Furthermore, the method of the present invention for designing, identifying, evaluating or searching an effector may further comprise the steps of contacting the dipeptidyl peptidase IV with a candidate compound, and thereafter measuring the activity of the dipeptidyl peptidase IV. When the dipeptidyl peptidase IV activity increases or decreases, it would be an index showing that the candidate compound is a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV.

The dipeptidyl peptidase IV activity can be measured by, for example, incubating a 1.5 ml reaction mixture [composition: 1.5 mM substrate

(Gly-Pro-paranitroanilide), 71 mM glycine-NaOH (pH 8.7)] at 37°C for 10 minutes in the presence of a candidate compound, and measuring the liberated paranitroanilide at the absorbance of 405 nm. During the measurement of the activity, the candidate compound may be evaluated by using a reaction system in  
5 which a suitable dilution series of the compound is added thereto.

The method of the present invention for designing, identifying, evaluating or searching the effector can be performed by, for example, sequentially selecting the interaction between the dipeptidyl peptidase IV and the compounds in a database in a computer to which the structures of plural of compounds had  
10 been inputted, or the interaction between the dipeptidyl peptidase IV and the designed compound, by visual methods (visual selection method) utilizing the database; and/or sequentially calculating the avidity with a computer, and searching a compound capable of stably interacting with the dipeptidyl peptidase IV from the database (computer-assisted avidity evaluation method) and the like,  
15 based on the three-dimensional structural coordinate of the present invention.

In the above visual selection method, the database of the structures of compounds may be a database in which the three-dimensional structural coordinates have been determined and inputted. Alternatively, in the case of a compound having a low molecular weight, the database may be a database in  
20 which the information for chemical covalent bond of a compound having a low molecular weight had been inputted, because the conformation can be relatively freely changed, and the three-dimensional structural coordinate of each conformation can be derived by calculation in a relatively short time.

Concretely, in the visual selection method, the expected complex between  
25 the dipeptidyl peptidase IV and a candidate compound or a part thereof is firstly

displayed on a computer screen, based on the three-dimensional structural coordinate of the present invention. Next, the intermolecular interaction binding between a compound in the database and the binding regions of the dipeptidyl peptidase IV is simulated on the computer, taking chemical interaction into consideration. Also, the simulation of the chemical modification of the compound is performed on the computer, and the changes in the interaction caused as a result thereof are observed on the computer screen. During the simulation, the three-dimensional space can be more easily understood by displaying the three-dimensional structure of the protein on the computer screen so that the structure corresponds to Crystal Eye glasses supplied by Silicone Graphics; simultaneously displaying two screens in which each angle is adjusted for displaying the object, according to the visual fields of the right eye and left eye, which is so-called referred to as "stereovision" which is frequently used by one of ordinary skill in the art; or the like. In addition, the three-dimensional structure can be visually studied by methods other than the stereoscopic displaying of the three-dimensional structure.

The candidate compound capable of generating suitable interaction can be obtained by displaying on a computer a group of candidates with appropriate conformation and selecting an appropriate one therefrom; calculating a structure having a low energy state on a computer; or the like. Next, a derivative of a compound capable of generating more preferable binding with the dipeptidyl peptidase IV may be searched among the candidate compound.

More specifically, on the level of the three-dimensional structure, the followings may be taken into consideration:

1 a group likely to be charged negatively, such as carboxyl group, nitro

- group, or a halogen group in the compound interacts with an amino acid residue having a positive charge, such as lysine, arginine or histidine in the dipeptidyl peptidase IV;
- 2 a group likely to be charged positively, such as amino group, imino group  
5 or guanidyl group in the compound interacts with an amino acid residue having negative charge, such as glutamic acid or aspartic acid in the dipeptidyl peptidase IV;
- 3 a hydrophobic functional group such as an aliphatic group or an aromatic group in the compound interacts with a hydrophobic amino acid residue  
10 such as alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophane or methionine in the dipeptidyl peptidase IV;
- 4 a group involved in hydrogen bonding, such as hydroxyl group or amide group is allowed to form hydrogen bonding with a main chain or side chain portion;
- 15 5 a group or an atom likely to be charged negatively, such as carboxyl group, nitro group or a halogen group in the compound interacts with a positively charged atom on a main chain or side chain portion;
- 6 a group or an atom likely to be charged positively, such as amino group, imino group or guanidyl group in the compound interacts with a negative  
20 charged atom on a main chain or a side chain portion;
- 7 the flexibility of the three-dimensional structure of the compound is lowered by, for instance, cyclizing the linear chain portion;
- or the like. For example, a derivative may be designed and synthesized so that the atoms having negative charge of the candidate compound are located in the  
25 adjacent region of the side chain of an amino acid residue having positive charge

such as lysine, arginine or histidine, in the amino acid residue of the dipeptidyl  
peptidase IV, and that an atom having positive charge of the candidate  
compound is located in the adjacent region of the side chain of the amino acid  
residue having negative charge such as glutamic acid or aspartic acid in the  
5 amino acid residue of the dipeptidyl peptidase IV. Also, a group suitable for  
forming a hydrophobic interaction may be introduced into the portion capable of  
forming a hydrophobic interaction between the compound and the dipeptidyl  
peptidase IV, to design and synthesize a derivative. In addition, a group suitable  
for forming hydrogen bonding may be introduced into the portion capable of  
10 forming hydrogen bonding between the compound and the dipeptidyl peptidase  
IV, to design and synthesize a derivative. In the above-mentioned designing, it is  
desirable that van der Waals interaction is as high as possible, and that steric  
hindrance does not occur between each of the atoms. Furthermore, it is desirable  
that new void portions are not produced by modification of the compound and  
15 that in regions already containing void portions, the void portions are filled as  
much as possible.

As described above, the design, identification, evaluation or searching of a  
final compound can be thus performed with visually comprehensively  
considering intermolecular interaction and other factors on a computer screen.

20 In the computer-assisted avidity evaluation method, in order to determine  
the validity for the designing of a new compound, and to obtain a compound that  
can stably interact from the compounds in the database, a docking software  
(DOCK, GOLD, FlexX, Glide or the like) is used for evaluation of binding based  
on the energy by calculating a molecular force field between the compound and  
25 the dipeptidyl peptidase IV, evaluation of binding based on chemical

characteristics, evaluation of binding based on the Protein Data Bank (PDB), and the like. Further, in a model system consisting of the compound and the dipeptidyl peptidase IV, or in a model system further comprising solvent molecules and the like, it can be led to a compound that can stably interact by obtaining the index showing avidity, such as free energy of bonding, the ratio obtained from bond state number and non-bond state number, and the like by using molecular kinetic calculation or Monte Carlo calculation. The programs for calculation of molecular force field and molecular kinetic include AMBER, CHARMm, DISCOVER, PRESTO and the like, and the force field used includes AMBER, CHARMm, OPLS, MMCF, CVFF and the like. Furthermore, a program such as Ludi which automatically outputs the candidates for a candidate compound by providing a three-dimensional structural coordinate of the amino acid residues interacting in the dipeptidyl peptidase IV may be used.

The visual selection method and computer-assisted avidity evaluation method can be performed alone or in combination. In the case of performing the methods in combination, the avidity is actually calculated for the compounds that has been expected to be more desirable in visual investigation, and the validity thereof is evaluated. By repeatedly performing the calculation and evaluation, more excellent compounds may be designed, identified, evaluated or searched.

Next, the designed, identified, evaluated or searched compound is optimized to be a more excellent compound, such as a compound having more excellent characteristics as a medicament, such as being excellent *in vivo* kinetics, having low toxicity and low side-effect; a compound having a still higher biological activity as an effector; a compound having an advantageous structure as a medicament in view of its oral administration; and the like.

The resulting candidate compound can be obtained using generally used techniques for chemical synthesis depending on the kind of the compound.

The present invention also encompasses an effector of the dipeptidyl peptidase IV, which is obtained by the method of the present invention for  
5 designing, identifying, evaluating or searching an effector. When the effector is a compound capable of inhibiting or enhancing the activity of the dipeptidyl peptidase IV, the effector (inhibitor or activator) is expected to be an agent for, for example, a modulatory agent of immune response, a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease,  
10 chronic rheumatoid arthritis, AIDS, cancer and the like.

The three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention can be provided as a computer program, a medium or the like, which displays the three-dimensional structure of the molecule based on the three-dimensional structural coordinate and can be provided via a  
15 telecommunication line or the like. Therefore, using a computer or the like, the three-dimensional coordinate of the dipeptidyl peptidase IV can be displayed in detail, allowing to perform the method of the present invention for designing, identifying, evaluating or searching an effector more rapidly, conveniently and logically.

20 The present invention also encompasses a program or a medium therefor for use of the three-dimensional structural coordinate, in which all and/or a part of the three-dimensional structural coordinate of the dipeptidyl peptidase IV of the present invention is recorded.

The medium may be any of those in which the three-dimensional  
25 structural coordinate of the present invention can be derived on a program that

runs on a computer, and includes, for instance, electric memory media referred to as memory; semi-permanent memory media such as a FD, a hard disk, an optical disk, an opto-magnetic disk and a magnetic tape, and the like. In addition, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention also encompass those having a form which can be communicated via a telecommunication line such as internet.

Also, the program and the medium therefor for use of the three-dimensional structural coordinate of the present invention may further comprise a means for displaying the three-dimensional graphic display of the molecule.

10 The program or the medium therefor which comprises the means for displaying the three-dimensional graphic display has advantages that visual studies and/or calculation of avidity can be made more conveniently, so that there is more facilitated a logical design on the three-dimensional structural level for obtaining a compound having excellent characteristics such as higher avidity, higher

15 biological activity, higher biological stability, higher thermomechanical stability, higher absorbency to a living body, and lower toxicity than those for known effectors of the dipeptidyl peptidase IV.

As the means capable of displaying the three-dimensional graphic display, there may be generally used a program that is made so that a means for inputting

20 the three-dimensional structural coordinate of the molecule, a means for measuring visual representation of the coordinate on a computer screen, the distance between the represented atoms in the molecule, bond angles or the like, a means for addition or modification of the coordinate, and the like can be provided. Furthermore, there may be used a program that has been made so that

25 a means for calculating the structure energy of the molecule based on the

coordinate of the molecule, a means for calculating the free energy of bonding, and the ratio of bonding state number to non-bonding state number in consideration of solvent molecules such as water molecule can be provided.

Examples of the program suitable for such purposes include Insight II,

5 QUANTA and the like, which are computer programs commercially available from Accelrys Inc., and the present invention is not limited to these programs. Also, the above-mentioned programs can be introduced into a computer referred to as a work station supplied from Silicone Graphics Inc., SunMicro-Systems Ltd., or the like, and used.

10 According to the crystal of dipeptidyl peptidase IV of the present invention, there can be exhibited excellent effects that the three-dimensional structural coordinate can be obtained as an information for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV useful as a

15 modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and that the crystal of a complex of the dipeptidyl peptidase IV and a known effector can be readily prepared.

Also, according to the three-dimensional structural coordinate of the present invention, there is exhibited an excellent effect that the effector can be designed,

20 identified, evaluated or searched. In addition, according to the method for obtaining a three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of the present invention, there is exhibited an excellent effect that the three-dimensional structural coordinate of the homolog protein of the dipeptidyl peptidase IV of which three-dimensional structure is unknown can

25 be conveniently and rapidly provided. Furthermore, according to the method for

obtaining a three-dimensional structure of a crystal of a complex of the dipeptidyl peptidase IV of the present invention and an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. Moreover, according to the method of the present invention for identifying a pharmacophore of the dipeptidyl peptidase IV and the effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can provide a target for designing the effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability, and higher absorbency to a living body. According to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, there is exhibited an excellent effect that the method can logically and conveniently provide an effector useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and having excellent characteristics such as higher avidity, higher biological activity, higher biological stability, higher thermomechanical stability,

and higher absorbency to a living body. According to the effector of the dipeptidyl peptidase IV of the present invention, there are exhibited excellent effects that the effector is capable of modifying immune response and capable of treating or preventing diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Furthermore, according to the program and medium therefor of the present invention, there is exhibited an excellent effect that the method for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV can be performed more rapidly and conveniently.

The present invention will be hereinafter more specifically explained by the following Examples, but the present invention is not intended to be limited by the Examples in any way. Unless otherwise indicated, the reaction conditions, procedures and the like can be referred to the instruction manual attached to the reagents used, *Molecular Cloning A Laboratory Manual*, third edition, Sambrook et al. [issued by Cold Spring Harbor Laboratory Press (2001)], and the like.

Example 1 Construction of Recombinant Baculovirus for Expression of Soluble Human Dipeptidyl Peptidase IV

(1) Cloning of Soluble Human Dipeptidyl Peptidase IV (shDPPIV) cDNA

Caco-2 cells [provided by American Type Culture Collection (ATCC)] were cultured at 37°C using Dulbecco's Modified Eagle Medium (manufactured by Invitrogen) containing 20% by volume of inactivated fetal bovine serum (manufactured by Invitrogen; inactivated by incubation at 56°C for 30 minutes) and 1% by volume of nonessential amino acid (manufactured by Invitrogen), in

the presence of 5% by volume of CO<sub>2</sub>.

Next, total RNA was extracted from the Caco-2 cells obtained.

Extraction of the total RNA was carried out using a product manufactured by Nippon Gene Co. Ltd. under the trade name of ISOGEN in accordance with the attached instruction manual. The obtained total RNA was used as a template for RT-nested PCR method described below.

In order to obtain a nucleic acid corresponding to a soluble human DPPIV from which the signal peptide sequence was removed (amino acid nos: 33-766 of SWISS-PROT Accession No: P27487), first, a cDNA fragment sequence of human DPPIV gene was amplified by RT-nested PCR method with total RNA of the Caco-2 as a template.

The thermal profile in the PCR is 30 cycles of reaction, in which one cycle comprises denaturation at 94°C for 30 seconds, annealing at 55°C for 30 seconds and polymerase extension reaction at 72°C for 1 minute.

The amplified DNA fragment was separated by agarose gel electrophoresis method, and a small fragment of the gel of the corresponding band portions was cut out. Thereafter, the DNA fragment was extracted from the obtained small fragments of the gel using a product manufactured by Bio 101 under the trade name of GENE CLEAN SPIN Kit, and purified. The obtained fragment was inserted into vector pCR2.1-TOPO contained in TOPO TA Cloning (registered trade mark) Kit manufactured by Invitrogen to construct pCR-shDPPIV.

In order to confirm whether or not the obtained cDNA fragment encodes the desired polypeptide, deletion mutants regarding the DNA fragment having various lengths were prepared, and a nucleotide sequence for the DNA fragment

was determined as follows.

First, a DNA fragment having a size of 2.2 kbp obtained by double digestion of the pCR-shDPPIV with *Bam*HI and *Eco*RI was inserted into a corresponding restriction site in pUC19 (manufactured by Takara Bio Inc.), to  
5 construct a plasmid pUshDPPIV. Various deletion plasmids were prepared using the plasmid pUshDPPIV by a conventional method.

The nucleotide sequence for the DNA fragment was determined using the obtained deletion plasmid or plasmid pCR-shDPPIV, and a product manufactured by Perkin-Elmer Cetus Inc. under the trade name of Taq  
10 DyeDeoxy Terminator Cycle Sequencing Kit and Model 373S sequencer manufactured by Applied Biosystems.

Also, the amino acid sequence of the polypeptide encoded by the above-mentioned DNA fragment was determined on the basis of the nucleotide sequence.

15 The determined amino acid sequence was compared with the sequence for a full length DPPIV of human colon shown in SEQ ID NO: 2. As a result, it was confirmed that the corresponding regions (regions excluding the transmembrane region) were identical.

Thus, it was confirmed that the DNA fragment encodes the desired  
20 polypeptide shDPPIV, namely a polypeptide in which the transmembrane region (amino acid nos: 1-32 at N-terminal side) in the full-length human DPPIV was deleted and a polyhistidine peptide was added to the C-terminal side.

## (2) Preparation of Recombinant Baculovirus

25 Plasmid pUshDPPIV was digested with a restriction enzyme to give a

DNA fragment encoding shDPPIV gene. The obtained fragment was inserted into pAcGP67B (manufactured by BD PharMingen) to construct a baculovirus transfer vector pAcGP67B-shDPPIV.

5 Fifteen minutes before the transfection, Sf21 cells were washed twice with a TNM-FH medium comprising 10% by volume of fetal bovine serum. The Sf21 cells were then transferred to a well of a 6-well plate by  $2.4 \times 10^6$  cells per well.

10 Furthermore, 2 to 5  $\mu\text{g}$  of the baculovirus transfer vector and a 0.5  $\mu\text{g}$  linear baculovirus DNA (trade name: BaculoGold virus DNA, manufactured by BD PharMingen) were mixed, and the mixture was allowed to stand at room temperature for 5 minutes. Next, 1 ml of Transfection Buffer B (manufactured by BD PharMingen) was added to the obtained mixture, and the mixture was thoroughly mixed to give a Transfection Buffer B/DNA mixture.

15 The medium in the wells of the 6-well plate and the cells that had not been adhered to the wells were removed, and 1 ml of Transfection Buffer A (manufactured by BD PharMingen) was added to each of the wells. The Transfection Buffer B/DNA mixture was gradually added dropwise to the wells of the 6-well plate, with gently stirring the 6-well plate. The cells were incubated at 28°C for 4 hours in the wells of the 6-well plate. Thereafter, the  
20 transfection buffer was removed, and 3 ml of TNM-FH medium containing 10% by volume of fetal bovine serum was added to the wells of the 6-well plate. The cells were cultured at 28°C in each of the wells of the 6-well plate for 5 days, and the culture supernatant was collected. The culture supernatant was used for amplification of virus using Sf21 cells to give a virus stock solution.

## Example 2 Preparation and Crystallization of shDPPIV

### (1) Expression of shDPPIV in Insect Cells

Sf21 cells were cultured using a serum free medium EX-CELL 400 (manufactured by JRH Biosciences) and T flask, and Tn5 cells (provided by  
5 Invitrogen) were cultured using a serum free medium EX-CELL 401 (manufactured by JRH Biosciences) and a T flask, at 28°C, respectively. At the time when the proliferation of the cells reached 70% confluent, the old medium was removed, and a fresh medium was added at 40 ml per one 225-cm<sup>2</sup> flask. Then, 1.5 ml of virus stock solution after amplification for three times (having  
10 multiplicity of infection (MOI) of about 2) was added to the cells to infect the cells, and the cells were incubated at 28°C for 4 days. The culture supernatant four days after the infection was collected and stored at -20°C. The culture supernatant was used for the purification of shDPPIV protein as described below.

### 15 (2) Purification of shDPPIV Protein

In each step for the purification of shDPPIV, the activity of DPPIV was measured by incubating a 0.1 ml reaction mixture containing a 1.5 mM substrate [manufactured by Peptide Institute, Gly-Pro-paranitroanilide (pNA)], 71 mM Gly-NaOH (pH 8.7) and the DPPIV, and detecting the liberated pNA.  
20 Meanwhile, the reaction mixture was incubated at 37°C for 10 minutes. During the incubation, the absorbance at 405 nm was monitored.

Also, the protein concentration was quantified by using a product manufactured by Bio-Rad Laboratories, Inc. under the trade name of DC protein Assay Kit II.

25 The purity of the protein was confirmed by subjecting a protein sample

in each step to SDS-PAGE using 7.5% polyacrylamide gel according to the method by Laemmli et al.

The culture supernatant stored at -20°C in the above-mentioned (1) was melted at 4°C and filtered with a bottle top filter (manufactured by Becton, Dickinson and Company) or with 0.45 µm filter (KURABO INDUSTRIES LTD.) to remove insoluble materials. The supernatant after the filtration was concentrated to an about tenth volume by using a concentrator Vivaflow 50 (manufactured by Sartorius AG) or Amicon stirrer cell model 8400 (manufactured by Millipore Corporation) to give a concentrated solution.

The obtained concentrated solution was dialyzed against buffer A (20 mM HEPES-NaOH, 0.5 M NaCl, pH 8.0) at 4°C overnight, and applied to a nickel column [one in which nickel was immobilized to HiTrap Chelating column (trade name, manufactured by Amersham-Pharmacia) (5 ml × 2)] equilibrated with buffer A. The column was washed with 10 column volumes of buffer A, and then with buffer A containing 50 mM imidazole. The elution of the fraction containing shDPPIV was carried out by a linear gradient of 50 to 500 mM imidazole. The fraction found to have DPPIV activity was collected, and dialyzed overnight at 4°C against buffer B (20 mM HEPES-NaOH, pH 8.0, 50 mM NaCl). After the dialysis, the sample was purified by using an anion exchange column [manufactured by Amersham-Pharmacia under the trade name: Resource Q (6 ml)] equilibrated with buffer B. The column was washed with buffer B, and thereafter shDPPIV was eluted by a linear gradient of 15 column volumes of 50 to 500 mM NaCl. The fractions found to have DPPIV activity were collected, and used as a purified preparation.

(3) Preparation of Protein Sample for Crystallization

The shDPPIV purification sample (9 ml) obtained in the above (2) was concentrated using a product manufactured by Millipore Corporation under the trade name of Centricon 10 until the protein concentration reached 10 mg/ml.

5 The obtained product was used as a protein sample for crystallization. The protein sample for crystallization was stored at 4°C.

A precipitation agent solution containing 0.18 M glycine-NaOH (pH 9.5), 0.18 M sodium sulfate and 18% by weight of PEG4000, and a 10 mg/ml dipeptidyl peptidase IV solution were mixed, and thereafter, a drop of the  
10 obtained mixed solution was placed on a product under the trade name of Cryschem Plate (manufactured by Hampton Research). The above-mentioned precipitation solution was allowed to stand at 20°C as a reservoir solution to allow crystallization.

15 (4) Crystallization of shDPPIV

The crystallization of shDPPIV was carried out by a sitting-drop method, which is one of vapor diffusion methods.

The formation of crystal was observed with the passage of time using a stereoscopic microscope. As a result, after about two weeks, a large crystal  
20 having a maximum size of 500  $\mu\text{m}$   $\times$  300  $\mu\text{m}$   $\times$  100  $\mu\text{m}$  was obtained. The crystal is also referred to as a native crystal. The microphotograph of the obtained crystal is shown in Figure 1. In Figure 1, the visual field is 4000  $\mu\text{m}$   $\times$  3000  $\mu\text{m}$ .

25 Example 3 Three-Dimensional Structural Analysis of Crystals

(1) X-ray Diffraction

The crystal obtained in Example 2 mentioned above was soaked in a cryoprotecting buffer [composition: 0.18 M glycine-NaOH (pH 9.5), 19% by weight of PEG4000, 0.18 M sodium acetate, 15% glycerol], and immediately thereafter the mixture was placed under nitrogen gas stream (100 K) to rapidly freeze the mixture.

The X-ray diffraction intensity data of the above crystal were collected up to the resolution of  $3.0\text{\AA}$  using a product manufactured by Rigaku International Corporation under the trade name of R-Axis IV in nitrogen gas stream (100 K), and converted to the structure factor using a program MOSFLM (Version 6.11). A photograph of the diffraction pattern is shown in Figure 2.

From the obtained diffraction intensity data, it was determined that the crystal form to which the crystal belongs was orthorhombic, that the space group was  $P2_12_12_1$ , and the lattice constants were  $a = 118.0 \pm 5.0\text{\AA}$ ,  $|b| = 125.9 \pm 5.0\text{\AA}$  and  $|c| = 136.8 \pm 5.0\text{\AA}$ .

(2) Multiple Isomorphous Replacement Method

In order to derive an electron density map, multiple isomorphous replacement method was carried out. The crystal obtained in Example 2 was soaked for 3 days and 4 days in a crystallization solution prepared by dissolving mercury chloride until being saturated, to give two different kinds of isomorphous replacement crystals containing mercury atoms in the crystals. The X-ray diffraction intensity data were collected in the same manner as those for the native crystals.

In the determination of the phase in the structural analysis, CCP4

(Collaborative Computational Project, Number 4, 1994. "The CCP4 Suite: Programs for Protein Crystallography," *Acta Cryst. D* 50, 760-763) program was used.

5 First, Fourier transform calculation utilizing the difference between the diffraction intensity obtained from the two kinds of isomorphous replacement crystals of mercury and the diffraction intensity obtained from the native crystal was performed using MLPHARE contained in the CCP program package. The position of each mercury atom in the unit cell of the real space was determined by investigating large peaks provided by heavy atoms (mercury) in the obtained  
10 Patterson's diagram. The phase of the crystal structure factor of the native crystals was determined by using the obtained position coordinate of mercury atoms. Furthermore, in order to determine the coordinate of each mercury atom more accurately using DM and SOLOMON contained in the CCP program package, refinement was carried out using three crystal structure factors of the  
15 native crystals and of the two kinds of mercury isomorphous replacement crystals.

An electron density map of the crystals of the dipeptidyl peptidase IV in real space was obtained using the phase of the crystal structure factor of the native crystals calculated from the refined coordinates of the mercury atoms.  
20 Furthermore, the electron density map was improved by carrying out smoothening and histogram matching of the electron density map in a solvent region, to obtain an electron density map critical for molecular modeling.

### (3) Molecular Modeling

25 The sites corresponding to the amino acid residues of the dipeptidyl

peptidase IV were identified on the electron density map by using QUANTA (manufactured by Accelrys, Inc.), to build molecular models.

As expected from the lattice constants, there were two molecules of the dipeptidyl peptidase IV in an asymmetry unit, and a model was built for each of the molecules. The refinement of the obtained molecular model was carried out using CNX (manufactured by Accelrys, Inc.), and the molecular model was adjusted again using the QUANTA for the obtained improved electron density map. The procedures were repeated to build a more accurate molecular model. In the refinement of the final coordinate, diffraction intensity data measured again were used after OSMIC confocal mirror (manufactured by Rigaku International Corporation) had been introduced into R-AXIS IV (trade name, manufactured by Rigaku International Corporation).

As a result, the resolution was improved from the previous 3.0Å to 2.6Å. Furthermore, 273 molecules of bound water and 5 molecules of N-acetyl glucosamine residues per molecule of the dipeptidyl peptidase IV were identified in an asymmetric unit. R factor, which is an index for accuracy of the obtained molecular model, was 24.89%, and a free R factor, which independently was not taken into account of the calculation of refinement at the step of refinement, was 30.15%. During the procedure, the deviation of the interatomic bond distance (rms-deviation) and the bond angle from the ideal state of the three-dimensional structure were 0.006Å and 1.305°, respectively. The stereogram of the three-dimensional structure model of the crystals is shown in Figure 3, and the coordinate is shown in Figure 4. The present coordinate data were registered in PDB (Brookhaven Protein Data Bank) [PDB Code No: 1J2E, RSCB code No: 005544].

Here, as to those regions which did not take a regular structure in the crystals (in the disordered state), namely, the region from Asp 38 to that closer to the N-terminal side thereof, and the region for the tagged peptide (polyhistidine peptide) of the C-terminal side, the molecular model could not be built.

5 Furthermore, a part of the side chains projected to the surface of the molecules did not take a regular structure. However, these residues were not portions that play an important role for the function of enzymes.

In the three-dimensional structure of the dipeptidyl peptidase IV, which has been clarified by the Examples, it has been revealed that the amino acid  
10 residue involved in the activity deduced by various experiments for the dipeptidyl peptidase IV, namely, Ser 630, Asp 708 and His 740, form hydrogen bonds between the O<sub>δ2</sub> atom of Asp 708 and N<sub>δ1</sub> atom of His 740, and with the N<sub>ε2</sub> atom of His 740 and O<sub>γ</sub> atom of Ser 630, even the residues locate in distant locations on the primary sequence. Therefore, for the structural coordinate of  
15 Figure 4 and the three-dimensional structure model defined by the structural coordinate, it is suggested that the regions characterized by Ser 630, Asp 708 and His 740, and the whole or a part of amino acid residues that are located in the vicinity of Ser 630, Asp 708 and His 740 play an important role on the exhibition of the activity for the dipeptidyl peptidase IV and binding or interaction of the  
20 dipeptidyl peptidase IV with the effector, and that the compound matching the three-dimensional structure of the regions affect the activity for the dipeptidyl peptidase IV.

The present invention may be embodied in other various forms without  
25 departing from the spirit or essential characteristics thereof. The present

embodiment is therefore to be considered in all respects as illustrative and not restrictive, the scope of the invention being indicated by the appended claims rather than by the foregoing description and all changes which come within the meaning and range of equivalency of the claims are therefore intended to be embraced therein.

#### INDUSTRIAL APPLICABILITY

According to the crystal of the dipeptidyl peptidase IV of the present invention, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Also, according to the three-dimensional structure coordinate, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like can be obtained. Further, according to the method of the present invention for obtaining a three-dimensional structure coordinate of a homolog protein of a dipeptidyl peptidase IV, the refinement of the three-dimensional structure coordinate of the homolog protein of the dipeptidyl peptidase IV can be more conveniently carried out. Moreover, according to the method of the present invention for obtaining a three-dimensional structure coordinate of a crystal of a complex of a dipeptidyl

peptidase IV with an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Also, according to the method for identifying a pharmacophore of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body, and which can favorably act on the dipeptidyl peptidase IV can be obtained. Further, according to the method of the present invention for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, the information of a three-dimensional structure coordinate suitable for designing, identifying, evaluating or searching an effector of the dipeptidyl peptidase IV, which is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like, and is excellent in avidity, biological activity, biological stability, absorbency to a living body,

and which can favorably act on the dipeptidyl peptidase IV can be logically and conveniently obtained. In addition, the effector of the dipeptidyl peptidase IV of the present invention is useful as a modulatory agent of immune response and as a therapeutic or prophylactic agent for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like. Further, according to the program or the medium therefor of the present invention, the design, identification, evaluation and search for an effector of a dipeptidyl peptidase IV can be carried out rapidly and conveniently. Therefore, the present invention can be utilized in modulation of immune response and the treatment or prevention for diabetes, inflammation, multiple sclerosis, Graves' disease, chronic rheumatoid arthritis, AIDS, cancer and the like.

CLAIMS

1. A crystal of a dipeptidyl peptidase IV, having characteristics sufficient to ensure a resolution capable of analyzing its three-dimensional structure up to the side chain level by X-ray crystallographic structural analysis.

2. The crystal according to claim 1, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

3. The crystal according to claim 1 or 2, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added to a C-terminal side or N-terminal side thereof.

4. The crystal according to any one of claims 1 to 3, wherein the crystal has a space group of  $P2_12_12_1$ , and a lattice constant of the unit cell of  $|a| = 118.0 \pm 5.0 \text{ \AA}$ ,  $|b| = 125.9 \pm 5.0 \text{ \AA}$ ,  $|c| = 136.8 \pm 5.0 \text{ \AA}$ , and  $\alpha = \beta = \gamma = 90^\circ$ , and is orthorhombic.

5. The crystal according to any one of claims 1 to 4, wherein the crystal has the structural coordinate shown in Figure 4.

6. The crystal according to any one of claims 1 to 4, wherein the crystal has a structural coordinate different from the structural coordinate as shown in

Figure 4 via fluctuation of a protein.

7. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising the structural coordinate shown in Figure 4.

5

8. A three-dimensional structural coordinate of a dipeptidyl peptidase IV, comprising a structural coordinate different from the structural coordinate as shown in Figure 4 via fluctuation of a protein.

10 9. The three-dimensional structural coordinate according to claim 8, wherein the fluctuation of a protein is a state that is caused by molecular oscillation or temperature, and exhibits an activity for the dipeptidyl peptidase IV in a living body.

15 10. The three-dimensional structural coordinate according to any one of claims 7 to 9, wherein the dipeptidyl peptidase IV is a soluble polypeptide comprising a region located at extramembrane in a full-length human dipeptidyl peptidase IV.

20 11. The three-dimensional structural coordinate according to any one of claims 7 to 10, wherein the dipeptidyl peptidase IV is a polypeptide having an amino acid sequence in which a transmembrane region is deleted from the amino acid sequence of SEQ ID NO: 2, and a tag peptide is optionally added of to a C-terminal side or N-terminal side thereof.

25

12. A three-dimensional structural coordinate of a region in a dipeptidyl peptidase IV, comprising the three-dimensional structural coordinate of the region selected from the group consisting of the following (a) to (d):

(a) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid  
5 sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues located in the adjacent area of each of the Ser 630, Asp 708 and His 740 in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate;

10 (b) a region characterized by Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of amino acids in the group of the amino acid residues  
15 located in the adjacent area of each of Ser 630, Asp 708 and His 740, in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural coordinate,

(c) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics  
20 physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and

all or a part of a group of the amino acid residues located adjacent area of said group of the amino acid residues in the structural coordinate shown in Figure 4 or the three-dimensional structure model defined by the structural  
25 coordinate; and

- (d) a region characterized by a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of Ser 630, Asp 708 and His 740 in the amino acid sequence of SEQ ID NO: 2, and
- 5 all or a part of a group of amino acid residues comprising amino acids capable of maintaining physicochemical characteristics physiologically equivalent to each of the amino acids in the group of the amino acid residues located in the adjacent area of said group of the amino acids, in the structural coordinate shown in Figure 4 or the three-dimensional
- 10 structure model defined by the structural coordinate,
- wherein the region in the dipeptidyl peptidase IV is a region involved in binding or interaction between the dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV.
- 15 13. The three-dimensional coordinate according to claim 12, wherein the physicochemical characteristic is selected from the group consisting of features in shape of a three-dimensional structure, hydrophobicity, electric charge and pK.
14. A method for obtaining a three-dimensional coordinate of a homolog
- 20 protein of a dipeptidyl peptidase IV, characterized in refining an electron density map of the homolog protein of the dipeptidyl peptidase IV comprising the amino acid sequence of SEQ ID NO: 2, based on all and/or a part of the three-dimensional coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.

15. A method for obtaining a three-dimensional structural coordinate of a crystal of a complex of a dipeptidyl peptidase IV and an effector of the dipeptidyl peptidase IV characterized in using all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, to give a three-dimensional structural coordinate.

16. A method for identifying pharmacophore of an effector of the dipeptidyl peptidase IV, characterized in identifying the pharmacophore based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13, and the steric conformation of the effector of the dipeptidyl peptidase IV.

17. A method for designing, identifying, evaluating or searching an effector of a dipeptidyl peptidase IV, characterized in designing, identifying, evaluating or searching a compound capable of acting on the dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13.

18. The method according to claim 17, wherein the method for designing, identifying, evaluating or searching an effector comprises the steps of:

(i) identifying a region to be targeted for binding or interaction with the effector in a dipeptidyl peptidase IV, based on all and/or a part of the three-dimensional structural coordinate according to any one of claims 7 to 13 and the steric conformation of the effector of the dipeptidyl peptidase IV;

(ii) identifying atoms or atomic groups capable of generating in the above

region at least one intermolecular interaction selected from the group consisting of covalent bond, ionic interaction, ion-dipole interaction, dipole-dipole interaction, hydrogen bonding, van der Waals force, electrostatic interaction and hydrophobic interaction, with the atoms or atomic groups existing in a candidate compound; and

(iii) designing a compound based on the information of the above step (i) and/or (ii).

19. The method according to claim 18, wherein the method further comprises the steps of:

detecting an interaction between the dipeptidyl peptidase IV and the designed, identified, evaluated or searched candidate compound, wherein when an interaction is detected, the candidate compound is identified as a compound capable of binding to the dipeptidyl peptidase IV, based on a degree of the interaction as an index.

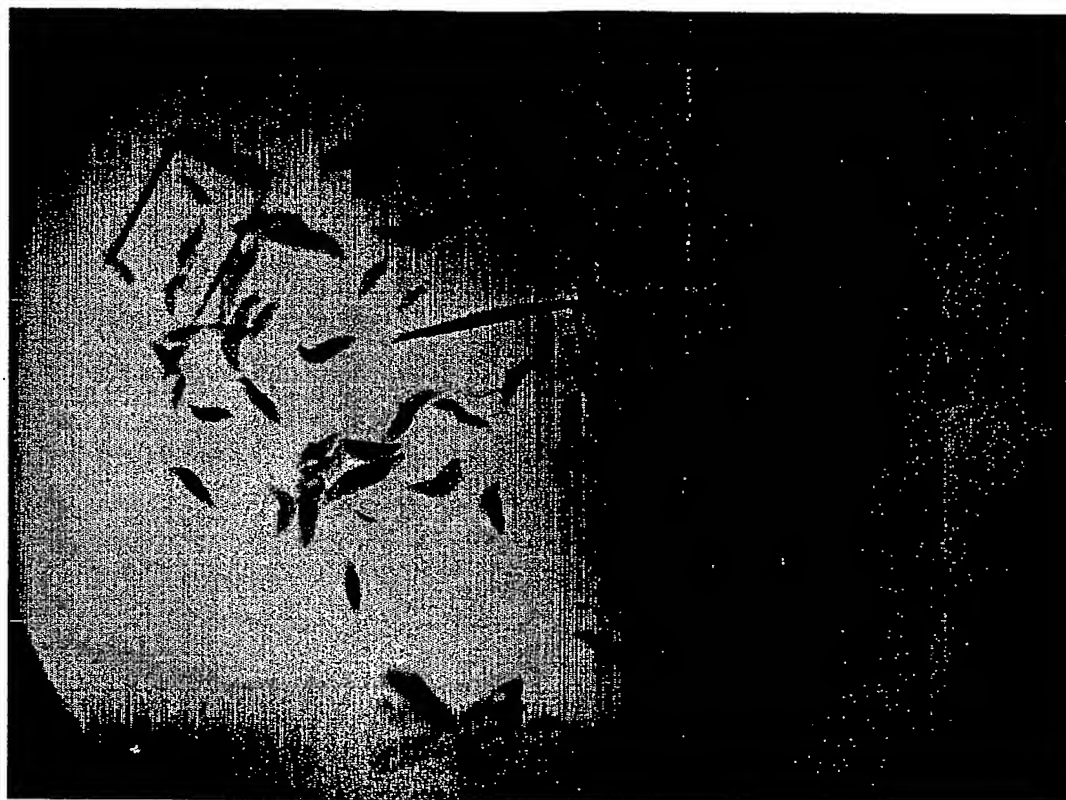
20. The method according to claim 18 or 19, wherein the method further comprises the steps of:

contacting the dipeptidyl peptidase IV with the designed, identified, evaluated or searched candidate compound and measuring an activity of the dipeptidyl peptidase IV, wherein when an activity increases or decreases, the designed, identified, evaluated or searched candidate compound is identified as a compound having enhancing action or inhibitory action on the activity of the dipeptidyl peptidase IV, based on a degree of the increase or decrease as an index.

21. An effector of the dipeptidyl peptidase IV obtainable by the method of any one of claims 17 to 20.
- 5 22. A program and a medium therefor for use of the three-dimensional structural coordinate of any one of claims 7 to 13, wherein all and/or a part of the three-dimensional structural coordinate of any one of claims 7 to 13 is recorded.
- 10 23. The program and the medium according to claim 22, comprising a means for identifying, searching, evaluating or designing a compound capable of binding to the dipeptidyl peptidase IV or a compound having an enhancing action or inhibitory action on the activity for the dipeptidyl peptidase IV.
- 15 24. The program and the medium according to claim 23, further comprising a means for displaying a three-dimensional graphic display of a molecule.

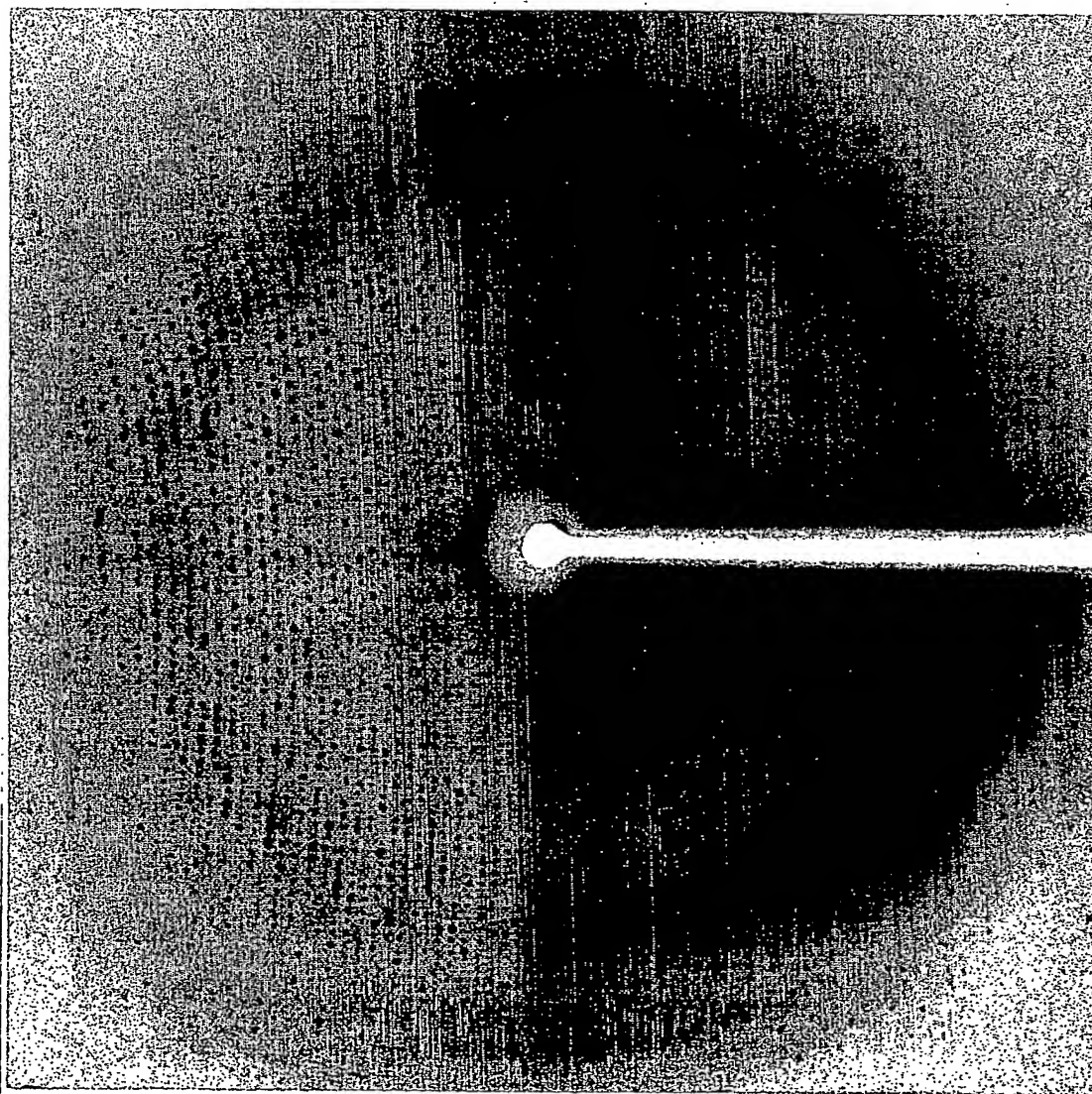
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FIG. 1



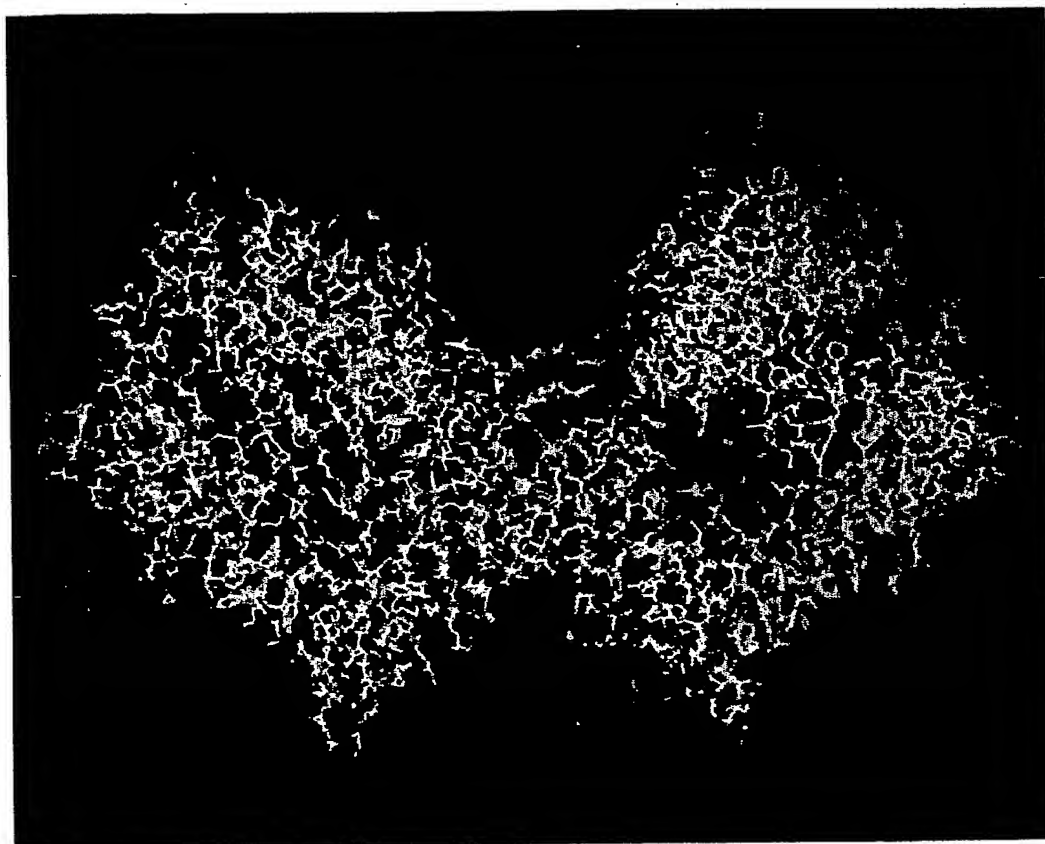
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FIG. 2



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FIG. 3



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## F I G. 4 - 1

Three-dimensional structural coordinate of dipeptidyl peptidase IV

ATOM	1	CB	ASP	38	44.493	31.885	58.927	1.00	42.46	A	C
ATOM	2	CG	ASP	38	44.146	32.095	57.467	1.00	42.00	A	C
ATOM	3	OD1	ASP	38	43.664	33.198	57.133	1.00	42.55	A	O
ATOM	4	OD2	ASP	38	44.360	31.171	56.655	1.00	40.85	A	O
ATOM	5	C	ASP	38	45.876	29.805	58.634	1.00	41.68	A	C
ATOM	6	O	ASP	38	46.980	30.327	58.778	1.00	42.02	A	O
ATOM	7	N	ASP	38	44.758	30.264	60.778	1.00	42.88	A	N
ATOM	8	CA	ASP	38	44.639	30.404	59.296	1.00	42.51	A	C
ATOM	9	N	SER	39	45.679	28.711	57.905	1.00	40.69	A	N
ATOM	10	CA	SER	39	46.775	28.013	57.241	1.00	39.98	A	C
ATOM	11	CB	SER	39	46.584	26.501	57.380	1.00	40.43	A	C
ATOM	12	OG	SER	39	45.410	26.079	56.703	1.00	41.11	A	O
ATOM	13	C	SER	39	46.960	28.343	55.763	1.00	39.60	A	C
ATOM	14	O	SER	39	47.870	27.813	55.123	1.00	39.66	A	O
ATOM	15	N	ARG	40	46.093	29.190	55.217	1.00	38.12	A	N
ATOM	16	CA	ARG	40	46.194	29.575	53.810	1.00	37.02	A	C
ATOM	17	CB	ARG	40	45.082	30.558	53.439	1.00	36.96	A	C
ATOM	18	CG	ARG	40	43.683	29.984	53.404	1.00	35.97	A	C
ATOM	19	CD	ARG	40	42.688	31.098	53.137	1.00	34.97	A	C
ATOM	20	NE	ARG	40	42.774	32.134	54.161	1.00	35.27	A	N
ATOM	21	CZ	ARG	40	42.097	33.276	54.125	1.00	35.55	A	C
ATOM	22	NH1	ARG	40	41.280	33.528	53.111	1.00	35.54	A	N
ATOM	23	NH2	ARG	40	42.239	34.167	55.097	1.00	34.68	A	N
ATOM	24	C	ARG	40	47.530	30.251	53.531	1.00	35.91	A	C
ATOM	25	O	ARG	40	48.100	30.901	54.407	1.00	34.18	A	O
ATOM	26	N	LYS	41	48.031	30.100	52.310	1.00	35.43	A	N
ATOM	27	CA	LYS	41	49.286	30.749	51.937	1.00	34.97	A	C
ATOM	28	CB	LYS	41	49.705	30.338	50.525	1.00	35.73	A	C
ATOM	29	CG	LYS	41	48.684	30.719	49.467	1.00	38.56	A	C
ATOM	30	CD	LYS	41	49.026	30.151	48.096	1.00	42.36	A	C
ATOM	31	CE	LYS	41	47.805	30.201	47.173	1.00	45.55	A	C
ATOM	32	NZ	LYS	41	48.070	29.686	45.791	1.00	47.41	A	N
ATOM	33	C	LYS	41	49.038	32.257	51.957	1.00	33.41	A	C
ATOM	34	O	LYS	41	47.891	32.715	51.981	1.00	33.24	A	O
ATOM	35	N	THR	42	50.110	33.032	51.954	1.00	31.47	A	N
ATOM	36	CA	THR	42	49.967	34.479	51.937	1.00	30.04	A	C
ATOM	37	CB	THR	42	50.860	35.139	53.000	1.00	31.23	A	C
ATOM	38	OG1	THR	42	52.234	34.843	52.725	1.00	30.79	A	O
ATOM	39	CG2	THR	42	50.501	34.622	54.386	1.00	30.12	A	C
ATOM	40	C	THR	42	50.389	34.971	50.558	1.00	28.34	A	C
ATOM	41	O	THR	42	50.977	34.220	49.782	1.00	27.76	A	O
ATOM	42	N	TYR	43	50.058	36.217	50.234	1.00	27.55	A	N
ATOM	43	CA	TYR	43	50.465	36.782	48.954	1.00	25.72	A	C
ATOM	44	CB	TYR	43	49.615	38.006	48.623	1.00	26.01	A	C
ATOM	45	CG	TYR	43	49.922	38.625	47.280	1.00	26.92	A	C
ATOM	46	CD1	TYR	43	50.977	39.527	47.130	1.00	26.68	A	C
ATOM	47	CE1	TYR	43	51.253	40.113	45.895	1.00	27.02	A	C
ATOM	48	CD2	TYR	43	49.152	38.315	46.158	1.00	26.40	A	C

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(Continued)

## FIG. 4 - 2

ATOM	49	CE2	TYR	43	49.424	38.891	44.919	1.00	25.89	A	C
ATOM	50	CZ	TYR	43	50.473	39.790	44.796	1.00	25.91	A	C
ATOM	51	OH	TYR	43	50.741	40.370	43.579	1.00	25.09	A	O
ATOM	52	C	TYR	43	51.933	37.165	49.160	1.00	24.97	A	C
ATOM	53	O	TYR	43	52.251	38.049	49.955	1.00	23.33	A	O
ATOM	54	N	THR	44	52.818	36.482	48.444	1.00	24.06	A	N
ATOM	55	CA	THR	44	54.255	36.685	48.580	1.00	25.90	A	C
ATOM	56	CB	THR	44	54.960	35.336	48.547	1.00	25.86	A	C
ATOM	57	OG1	THR	44	54.696	34.709	47.285	1.00	28.12	A	O
ATOM	58	CG2	THR	44	54.439	34.436	49.655	1.00	22.61	A	C
ATOM	59	C	THR	44	54.917	37.576	47.530	1.00	27.35	A	C
ATOM	60	O	THR	44	54.296	37.956	46.535	1.00	29.11	A	O
ATOM	61	N	LEU	45	56.191	37.894	47.765	1.00	27.39	A	N
ATOM	62	CA	LEU	45	56.978	38.722	46.853	1.00	26.43	A	C
ATOM	63	CB	LEU	45	58.377	38.954	47.425	1.00	26.07	A	C
ATOM	64	CG	LEU	45	59.310	39.860	46.612	1.00	26.21	A	C
ATOM	65	CD1	LEU	45	58.734	41.263	46.517	1.00	25.53	A	C
ATOM	66	CD2	LEU	45	60.672	39.896	47.266	1.00	24.37	A	C
ATOM	67	C	LEU	45	57.088	38.069	45.473	1.00	27.00	A	C
ATOM	68	O	LEU	45	56.939	38.740	44.449	1.00	27.84	A	O
ATOM	69	N	THR	46	57.354	36.766	45.445	1.00	26.70	A	N
ATOM	70	CA	THR	46	57.448	36.038	44.182	1.00	26.95	A	C
ATOM	71	CB	THR	46	57.838	34.559	44.407	1.00	26.87	A	C
ATOM	72	OG1	THR	46	59.150	34.495	44.966	1.00	31.74	A	O
ATOM	73	CG2	THR	46	57.833	33.793	43.110	1.00	28.08	A	C
ATOM	74	C	THR	46	56.076	36.091	43.517	1.00	26.96	A	C
ATOM	75	O	THR	46	55.965	36.094	42.289	1.00	25.36	A	O
ATOM	76	N	ASP	47	55.035	36.126	44.346	1.00	27.72	A	N
ATOM	77	CA	ASP	47	53.659	36.199	43.858	1.00	29.74	A	C
ATOM	78	CB	ASP	47	52.670	36.173	45.026	1.00	30.90	A	C
ATOM	79	CG	ASP	47	52.289	34.769	45.430	1.00	30.62	A	C
ATOM	80	OD1	ASP	47	51.778	34.595	46.553	1.00	32.28	A	O
ATOM	81	OD2	ASP	47	52.490	33.845	44.617	1.00	30.71	A	O
ATOM	82	C	ASP	47	53.477	37.482	43.073	1.00	28.87	A	C
ATOM	83	O	ASP	47	52.918	37.478	41.979	1.00	29.50	A	O
ATOM	84	N	TYR	48	53.945	38.581	43.648	1.00	28.54	A	N
ATOM	85	CA	TYR	48	53.859	39.878	42.994	1.00	29.04	A	C
ATOM	86	CB	TYR	48	54.191	40.991	43.996	1.00	27.50	A	C
ATOM	87	CG	TYR	48	54.448	42.333	43.354	1.00	25.16	A	C
ATOM	88	CD1	TYR	48	53.460	42.971	42.609	1.00	23.19	A	C
ATOM	89	CE1	TYR	48	53.703	44.184	41.982	1.00	24.84	A	C
ATOM	90	CD2	TYR	48	55.694	42.946	43.461	1.00	25.89	A	C
ATOM	91	CE2	TYR	48	55.956	44.165	42.838	1.00	26.76	A	C
ATOM	92	CZ	TYR	48	54.955	44.779	42.096	1.00	27.28	A	C
ATOM	93	OH	TYR	48	55.208	45.977	41.463	1.00	25.97	A	O
ATOM	94	C	TYR	48	54.820	39.953	41.796	1.00	28.80	A	C
ATOM	95	O	TYR	48	54.445	40.401	40.714	1.00	28.24	A	O
ATOM	96	N	LEU	49	56.054	39.499	41.988	1.00	29.41	A	N
ATOM	97	CA	LEU	49	57.046	39.552	40.918	1.00	30.39	A	C

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(Continued)

## FIG. 4 - 3

ATOM	98	CB	LEU	49	58.455	39.318	41.481	1.00	27.73	A	C
ATOM	99	CG	LEU	49	58.988	40.473	42.336	1.00	28.28	A	C
ATOM	100	CD1	LEU	49	60.438	40.223	42.711	1.00	26.99	A	C
ATOM	101	CD2	LEU	49	58.860	41.773	41.555	1.00	26.02	A	C
ATOM	102	C	LEU	49	56.804	38.606	39.752	1.00	30.71	A	C
ATOM	103	O	LEU	49	57.147	38.919	38.614	1.00	30.14	A	O
ATOM	104	N	LYS	50	56.198	37.459	40.024	1.00	32.51	A	N
ATOM	105	CA	LYS	50	55.959	36.491	38.971	1.00	33.54	A	C
ATOM	106	CB	LYS	50	56.289	35.098	39.485	1.00	33.30	A	C
ATOM	107	CG	LYS	50	57.763	34.940	39.790	1.00	33.89	A	C
ATOM	108	CD	LYS	50	58.591	35.213	38.545	1.00	35.19	A	C
ATOM	109	CE	LYS	50	60.071	34.945	38.778	1.00	38.12	A	C
ATOM	110	NZ	LYS	50	60.859	35.028	37.515	1.00	39.27	A	N
ATOM	111	C	LYS	50	54.572	36.517	38.361	1.00	34.93	A	C
ATOM	112	O	LYS	50	54.272	35.719	37.478	1.00	35.13	A	O
ATOM	113	N	ASN	51	53.731	37.436	38.822	1.00	36.66	A	N
ATOM	114	CA	ASN	51	52.379	37.569	38.294	1.00	38.39	A	C
ATOM	115	CB	ASN	51	52.428	37.859	36.791	1.00	41.61	A	C
ATOM	116	CG	ASN	51	53.407	38.968	36.436	1.00	44.75	A	C
ATOM	117	OD1	ASN	51	53.212	40.131	36.801	1.00	46.38	A	O
ATOM	118	ND2	ASN	51	54.470	38.609	35.717	1.00	45.80	A	N
ATOM	119	C	ASN	51	51.529	36.324	38.517	1.00	38.21	A	C
ATOM	120	O	ASN	51	50.708	35.976	37.674	1.00	40.60	A	O
ATOM	121	N	THR	52	51.720	35.647	39.641	1.00	36.74	A	N
ATOM	122	CA	THR	52	50.942	34.451	39.926	1.00	35.44	A	C
ATOM	123	CB	THR	52	51.297	33.888	41.298	1.00	35.57	A	C
ATOM	124	OG1	THR	52	52.646	33.415	41.272	1.00	38.62	A	O
ATOM	125	CG2	THR	52	50.367	32.750	41.666	1.00	35.25	A	C
ATOM	126	C	THR	52	49.431	34.686	39.869	1.00	35.17	A	C
ATOM	127	O	THR	52	48.699	33.889	39.276	1.00	36.44	A	O
ATOM	128	N	TYR	53	48.962	35.765	40.487	1.00	33.55	A	N
ATOM	129	CA	TYR	53	47.535	36.081	40.487	1.00	33.46	A	C
ATOM	130	CB	TYR	53	47.084	36.407	41.903	1.00	32.64	A	C
ATOM	131	CG	TYR	53	47.399	35.293	42.861	1.00	33.83	A	C
ATOM	132	CD1	TYR	53	48.341	35.462	43.872	1.00	34.11	A	C
ATOM	133	CE1	TYR	53	48.657	34.425	44.741	1.00	34.24	A	C
ATOM	134	CD2	TYR	53	46.775	34.050	42.741	1.00	36.17	A	C
ATOM	135	CE2	TYR	53	47.084	33.001	43.605	1.00	35.64	A	C
ATOM	136	CZ	TYR	53	48.026	33.199	44.601	1.00	35.74	A	C
ATOM	137	OH	TYR	53	48.343	32.170	45.453	1.00	35.79	A	O
ATOM	138	C	TYR	53	47.266	37.248	39.548	1.00	33.40	A	C
ATOM	139	O	TYR	53	47.486	38.404	39.895	1.00	33.56	A	O
ATOM	140	N	ARG	54	46.773	36.929	38.355	1.00	34.36	A	N
ATOM	141	CA	ARG	54	46.526	37.933	37.327	1.00	34.87	A	C
ATOM	142	CB	ARG	54	46.993	37.387	35.972	1.00	35.72	A	C
ATOM	143	CG	ARG	54	46.887	38.373	34.821	1.00	39.96	A	C
ATOM	144	CD	ARG	54	47.675	37.880	33.613	1.00	43.22	A	C
ATOM	145	NE	ARG	54	47.651	38.831	32.506	1.00	46.70	A	N
ATOM	146	CZ	ARG	54	46.587	39.068	31.744	1.00	49.10	A	C

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(Continued)

## FIG. 4 - 4

ATOM	147	NH1	ARG	54	45.451	38.416	31.968	1.00	49.25	A	N
ATOM	148	NH2	ARG	54	46.657	39.957	30.757	1.00	50.00	A	N
ATOM	149	C	ARG	54	45.100	38.445	37.202	1.00	33.84	A	C
ATOM	150	O	ARG	54	44.141	37.687	37.314	1.00	34.59	A	O
ATOM	151	N	LEU	55	44.982	39.748	36.966	1.00	33.05	A	N
ATOM	152	CA	LEU	55	43.693	40.402	36.788	1.00	32.40	A	C
ATOM	153	CB	LEU	55	43.792	41.892	37.123	1.00	29.74	A	C
ATOM	154	CG	LEU	55	44.042	42.344	38.557	1.00	32.26	A	C
ATOM	155	CD1	LEU	55	44.245	43.847	38.571	1.00	31.83	A	C
ATOM	156	CD2	LEU	55	42.857	41.967	39.448	1.00	33.66	A	C
ATOM	157	C	LEU	55	43.298	40.271	35.322	1.00	32.61	A	C
ATOM	158	O	LEU	55	44.004	40.769	34.441	1.00	33.62	A	O
ATOM	159	N	LYS	56	42.189	39.593	35.050	1.00	31.32	A	N
ATOM	160	CA	LYS	56	41.733	39.462	33.673	1.00	31.42	A	C
ATOM	161	CB	LYS	56	40.584	38.453	33.564	1.00	33.54	A	C
ATOM	162	CG	LYS	56	40.978	36.997	33.733	1.00	34.84	A	C
ATOM	163	CD	LYS	56	41.746	36.484	32.530	1.00	38.85	A	C
ATOM	164	CE	LYS	56	42.120	35.009	32.698	1.00	40.95	A	C
ATOM	165	NZ	LYS	56	43.117	34.537	31.685	1.00	43.33	A	N
ATOM	166	C	LYS	56	41.240	40.844	33.252	1.00	30.03	A	C
ATOM	167	O	LYS	56	40.839	41.648	34.088	1.00	28.24	A	O
ATOM	168	N	LEU	57	41.286	41.120	31.956	1.00	30.20	A	N
ATOM	169	CA	LEU	57	40.836	42.404	31.437	1.00	29.43	A	C
ATOM	170	CB	LEU	57	42.022	43.233	30.934	1.00	30.04	A	C
ATOM	171	CG	LEU	57	43.230	43.474	31.844	1.00	32.13	A	C
ATOM	172	CD1	LEU	57	44.123	44.524	31.194	1.00	29.05	A	C
ATOM	173	CD2	LEU	57	42.777	43.949	33.230	1.00	34.11	A	C
ATOM	174	C	LEU	57	39.911	42.132	30.271	1.00	28.16	A	C
ATOM	175	O	LEU	57	39.668	40.980	29.914	1.00	28.60	A	O
ATOM	176	N	TYR	58	39.394	43.196	29.676	1.00	26.69	A	N
ATOM	177	CA	TYR	58	38.530	43.050	28.518	1.00	25.82	A	C
ATOM	178	CB	TYR	58	37.071	42.890	28.934	1.00	25.51	A	C
ATOM	179	CG	TYR	58	36.195	42.420	27.797	1.00	26.86	A	C
ATOM	180	CD1	TYR	58	36.051	41.062	27.514	1.00	26.92	A	C
ATOM	181	CE1	TYR	58	35.294	40.631	26.429	1.00	26.28	A	C
ATOM	182	CD2	TYR	58	35.557	43.333	26.965	1.00	25.26	A	C
ATOM	183	CE2	TYR	58	34.803	42.911	25.882	1.00	26.13	A	C
ATOM	184	CZ	TYR	58	34.675	41.564	25.619	1.00	25.74	A	C
ATOM	185	OH	TYR	58	33.928	41.160	24.541	1.00	27.32	A	O
ATOM	186	C	TYR	58	38.681	44.288	27.647	1.00	24.95	A	C
ATOM	187	O	TYR	58	37.837	45.176	27.680	1.00	24.68	A	O
ATOM	188	N	SER	59	39.763	44.338	26.876	1.00	24.05	A	N
ATOM	189	CA	SER	59	40.037	45.470	25.997	1.00	24.31	A	C
ATOM	190	CB	SER	59	41.547	45.657	25.817	1.00	24.38	A	C
ATOM	191	OG	SER	59	42.187	45.931	27.051	1.00	28.99	A	O
ATOM	192	C	SER	59	39.405	45.294	24.628	1.00	23.54	A	C
ATOM	193	O	SER	59	39.795	44.420	23.860	1.00	24.84	A	O
ATOM	194	N	LEU	60	38.430	46.135	24.319	1.00	23.51	A	N
ATOM	195	CA	LEU	60	37.765	46.073	23.031	1.00	22.96	A	C

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(Continued)

## FIG. 4 - 5

ATOM	196	CB	LEU	60	36.256	45.910	23.228	1.00	21.27	A	C
ATOM	197	CG	LEU	60	35.528	46.977	24.048	1.00	20.80	A	C
ATOM	198	CD1	LEU	60	35.373	48.227	23.208	1.00	19.95	A	C
ATOM	199	CD2	LEU	60	34.159	46.466	24.488	1.00	18.91	A	C
ATOM	200	C	LEU	60	38.072	47.356	22.279	1.00	23.42	A	C
ATOM	201	O	LEU	60	38.507	48.340	22.869	1.00	23.10	A	O
ATOM	202	N	ARG	61	37.862	47.339	20.971	1.00	25.94	A	N
ATOM	203	CA	ARG	61	38.102	48.522	20.153	1.00	27.08	A	C
ATOM	204	CB	ARG	61	39.364	48.323	19.299	1.00	29.17	A	C
ATOM	205	CG	ARG	61	40.545	47.713	20.076	1.00	34.91	A	C
ATOM	206	CD	ARG	61	41.790	48.612	20.088	1.00	38.62	A	C
ATOM	207	NE	ARG	61	42.423	48.715	18.772	1.00	41.15	A	N
ATOM	208	CZ	ARG	61	43.337	47.871	18.299	1.00	41.78	A	C
ATOM	209	NH1	ARG	61	43.754	46.848	19.033	1.00	40.61	A	N
ATOM	210	NH2	ARG	61	43.821	48.042	17.076	1.00	43.39	A	N
ATOM	211	C	ARG	61	36.869	48.724	19.270	1.00	25.92	A	C
ATOM	212	O	ARG	61	36.616	47.939	18.358	1.00	26.31	A	O
ATOM	213	N	TRP	62	36.087	49.758	19.568	1.00	24.63	A	N
ATOM	214	CA	TRP	62	34.883	50.050	18.794	1.00	24.74	A	C
ATOM	215	CB	TRP	62	34.092	51.207	19.420	1.00	23.22	A	C
ATOM	216	CG	TRP	62	33.472	50.900	20.741	1.00	23.78	A	C
ATOM	217	CD2	TRP	62	32.302	50.110	20.972	1.00	23.80	A	C
ATOM	218	CE2	TRP	62	32.082	50.085	22.368	1.00	23.69	A	C
ATOM	219	CE3	TRP	62	31.416	49.419	20.133	1.00	22.71	A	C
ATOM	220	CD1	TRP	62	33.906	51.310	21.972	1.00	24.25	A	C
ATOM	221	NE1	TRP	62	33.075	50.824	22.955	1.00	23.12	A	N
ATOM	222	CZ2	TRP	62	31.013	49.396	22.945	1.00	23.91	A	C
ATOM	223	CZ3	TRP	62	30.357	48.736	20.703	1.00	24.08	A	C
ATOM	224	CH2	TRP	62	30.162	48.730	22.100	1.00	25.02	A	C
ATOM	225	C	TRP	62	35.241	50.427	17.365	1.00	25.48	A	C
ATOM	226	O	TRP	62	35.980	51.380	17.138	1.00	27.15	A	O
ATOM	227	N	ILE	63	34.722	49.682	16.398	1.00	26.16	A	N
ATOM	228	CA	ILE	63	35.000	49.991	15.003	1.00	25.88	A	C
ATOM	229	CB	ILE	63	35.312	48.727	14.180	1.00	25.95	A	C
ATOM	230	CG2	ILE	63	36.494	48.000	14.783	1.00	27.39	A	C
ATOM	231	CG1	ILE	63	34.092	47.810	14.138	1.00	24.70	A	C
ATOM	232	CD1	ILE	63	34.246	46.666	13.174	1.00	25.35	A	C
ATOM	233	C	ILE	63	33.788	50.680	14.400	1.00	26.00	A	C
ATOM	234	O	ILE	63	33.803	51.075	13.239	1.00	26.14	A	O
ATOM	235	N	SER	64	32.738	50.812	15.202	1.00	26.48	A	N
ATOM	236	CA	SER	64	31.510	51.470	14.768	1.00	28.43	A	C
ATOM	237	CB	SER	64	30.764	50.603	13.754	1.00	27.24	A	C
ATOM	238	OG	SER	64	30.181	49.481	14.392	1.00	28.00	A	O
ATOM	239	C	SER	64	30.597	51.727	15.964	1.00	29.08	A	C
ATOM	240	O	SER	64	31.008	51.606	17.119	1.00	26.71	A	O
ATOM	241	N	ASP	65	29.348	52.067	15.678	1.00	31.29	A	N
ATOM	242	CA	ASP	65	28.382	52.336	16.732	1.00	34.90	A	C
ATOM	243	CB	ASP	65	27.384	53.397	16.269	1.00	37.81	A	C
ATOM	244	CG	ASP	65	26.515	53.905	17.395	1.00	41.52	A	C

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(Continued)

## FIG. 4 - 6

ATOM	245	OD1	ASP	65	27.070	54.235	18.465	1.00	43.44	A	O
ATOM	246	OD2	ASP	65	25.281	53.986	17.211	1.00	44.76	A	O
ATOM	247	C	ASP	65	27.640	51.064	17.128	1.00	34.55	A	C
ATOM	248	O	ASP	65	26.753	51.091	17.981	1.00	33.76	A	O
ATOM	249	N	HIS	66	28.023	49.946	16.520	1.00	34.31	A	N
ATOM	250	CA	HIS	66	27.369	48.679	16.807	1.00	35.30	A	C
ATOM	251	CB	HIS	66	26.555	48.229	15.589	1.00	37.74	A	C
ATOM	252	CG	HIS	66	25.648	49.288	15.052	1.00	42.72	A	C
ATOM	253	CD2	HIS	66	24.298	49.393	15.056	1.00	44.80	A	C
ATOM	254	ND1	HIS	66	26.121	50.438	14.455	1.00	45.16	A	N
ATOM	255	CE1	HIS	66	25.101	51.206	14.114	1.00	46.24	A	C
ATOM	256	NE2	HIS	66	23.984	50.595	14.468	1.00	46.79	A	N
ATOM	257	C	HIS	66	28.314	47.555	17.223	1.00	33.78	A	C
ATOM	258	O	HIS	66	27.966	46.736	18.068	1.00	34.67	A	O
ATOM	259	N	GLU	67	29.502	47.501	16.635	1.00	31.93	A	N
ATOM	260	CA	GLU	67	30.432	46.434	16.979	1.00	31.45	A	C
ATOM	261	CB	GLU	67	30.557	45.463	15.801	1.00	31.46	A	C
ATOM	262	CG	GLU	67	30.356	46.103	14.447	1.00	33.17	A	C
ATOM	263	CD	GLU	67	30.357	45.092	13.311	1.00	35.48	A	C
ATOM	264	OE1	GLU	67	29.607	44.090	13.394	1.00	32.44	A	O
ATOM	265	OE2	GLU	67	31.104	45.306	12.329	1.00	36.60	A	O
ATOM	266	C	GLU	67	31.818	46.866	17.442	1.00	29.97	A	C
ATOM	267	O	GLU	67	32.240	48.003	17.241	1.00	30.44	A	O
ATOM	268	N	TYR	68	32.513	45.940	18.088	1.00	29.07	A	N
ATOM	269	CA	TYR	68	33.863	46.190	18.567	1.00	28.87	A	C
ATOM	270	CB	TYR	68	33.866	46.447	20.073	1.00	26.31	A	C
ATOM	271	CG	TYR	68	33.307	45.324	20.917	1.00	23.19	A	C
ATOM	272	CD1	TYR	68	32.000	45.376	21.400	1.00	21.93	A	C
ATOM	273	CE1	TYR	68	31.497	44.372	22.231	1.00	21.10	A	C
ATOM	274	CD2	TYR	68	34.102	44.232	21.281	1.00	23.23	A	C
ATOM	275	CE2	TYR	68	33.610	43.225	22.110	1.00	22.67	A	C
ATOM	276	CZ	TYR	68	32.304	43.305	22.582	1.00	22.02	A	C
ATOM	277	OH	TYR	68	31.810	42.321	23.403	1.00	22.72	A	O
ATOM	278	C	TYR	68	34.747	44.987	18.256	1.00	29.51	A	C
ATOM	279	O	TYR	68	34.244	43.885	18.028	1.00	28.32	A	O
ATOM	280	N	LEU	69	36.058	45.202	18.233	1.00	29.87	A	N
ATOM	281	CA	LEU	69	36.986	44.115	17.963	1.00	32.20	A	C
ATOM	282	CB	LEU	69	38.154	44.602	17.106	1.00	30.73	A	C
ATOM	283	CG	LEU	69	37.761	45.065	15.700	1.00	30.62	A	C
ATOM	284	CD1	LEU	69	38.978	45.629	14.963	1.00	29.98	A	C
ATOM	285	CD2	LEU	69	37.164	43.891	14.943	1.00	30.17	A	C
ATOM	286	C	LEU	69	37.492	43.588	19.292	1.00	34.73	A	C
ATOM	287	O	LEU	69	37.474	44.305	20.294	1.00	34.80	A	O
ATOM	288	N	TYR	70	37.927	42.334	19.305	1.00	37.39	A	N
ATOM	289	CA	TYR	70	38.423	41.726	20.528	1.00	42.16	A	C
ATOM	290	CB	TYR	70	37.251	41.359	21.444	1.00	42.66	A	C
ATOM	291	CG	TYR	70	37.689	40.866	22.799	1.00	43.06	A	C
ATOM	292	CD1	TYR	70	38.400	41.697	23.657	1.00	43.56	A	C
ATOM	293	CE1	TYR	70	38.837	41.253	24.892	1.00	44.69	A	C

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(Continued)

## FIG. 4 - 7

ATOM	294	CD2	TYR	70	37.421	39.563	23.213	1.00	43.93	A	C
ATOM	295	CE2	TYR	70	37.853	39.104	24.452	1.00	44.83	A	C
ATOM	296	CZ	TYR	70	38.563	39.959	25.286	1.00	45.17	A	C
ATOM	297	OH	TYR	70	39.004	39.532	26.516	1.00	47.21	A	O
ATOM	298	C	TYR	70	39.249	40.480	20.240	1.00	45.46	A	C
ATOM	299	O	TYR	70	38.976	39.752	19.287	1.00	46.31	A	O
ATOM	300	N	LYS	71	40.254	40.231	21.072	1.00	49.93	A	N
ATOM	301	CA	LYS	71	41.113	39.064	20.895	1.00	54.71	A	C
ATOM	302	CB	LYS	71	42.580	39.460	21.054	1.00	54.14	A	C
ATOM	303	CG	LYS	71	43.075	40.455	20.031	1.00	56.37	A	C
ATOM	304	CD	LYS	71	44.559	40.712	20.226	1.00	58.61	A	C
ATOM	305	CE	LYS	71	45.126	41.628	19.159	1.00	58.78	A	C
ATOM	306	NZ	LYS	71	46.590	41.830	19.361	1.00	60.82	A	N
ATOM	307	C	LYS	71	40.790	37.952	21.889	1.00	57.38	A	C
ATOM	308	O	LYS	71	41.109	38.062	23.075	1.00	58.38	A	O
ATOM	309	N	GLN	72	40.158	36.884	21.406	1.00	60.30	A	N
ATOM	310	CA	GLN	72	39.816	35.750	22.261	1.00	63.23	A	C
ATOM	311	CB	GLN	72	38.902	34.775	21.526	1.00	64.07	A	C
ATOM	312	CG	GLN	72	38.313	33.695	22.417	1.00	65.84	A	C
ATOM	313	CD	GLN	72	37.270	34.240	23.375	1.00	66.33	A	C
ATOM	314	OE1	GLN	72	36.251	34.790	22.952	1.00	67.19	A	O
ATOM	315	NE2	GLN	72	37.519	34.092	24.671	1.00	66.80	A	N
ATOM	316	C	GLN	72	41.122	35.049	22.607	1.00	65.34	A	C
ATOM	317	O	GLN	72	41.563	35.058	23.760	1.00	67.00	A	O
ATOM	318	N	GLU	73	41.736	34.442	21.597	1.00	66.09	A	N
ATOM	319	CA	GLU	73	43.012	33.763	21.775	1.00	67.12	A	C
ATOM	320	CB	GLU	73	43.008	32.420	21.046	1.00	68.53	A	C
ATOM	321	CG	GLU	73	41.974	31.433	21.570	1.00	71.35	A	C
ATOM	322	CD	GLU	73	42.223	31.026	23.012	1.00	72.71	A	C
ATOM	323	OE1	GLU	73	41.491	30.147	23.517	1.00	73.51	A	O
ATOM	324	OE2	GLU	73	43.147	31.585	23.643	1.00	74.16	A	O
ATOM	325	C	GLU	73	44.076	34.681	21.184	1.00	66.83	A	C
ATOM	326	O	GLU	73	44.563	35.592	21.857	1.00	67.65	A	O
ATOM	327	N	ASN	74	44.430	34.442	19.924	1.00	65.38	A	N
ATOM	328	CA	ASN	74	45.411	35.273	19.236	1.00	63.38	A	C
ATOM	329	CB	ASN	74	46.661	34.466	18.889	1.00	64.38	A	C
ATOM	330	CG	ASN	74	47.654	34.422	20.034	1.00	66.10	A	C
ATOM	331	OD1	ASN	74	48.128	35.463	20.496	1.00	65.51	A	O
ATOM	332	ND2	ASN	74	47.973	33.216	20.503	1.00	66.62	A	N
ATOM	333	C	ASN	74	44.794	35.859	17.977	1.00	61.55	A	C
ATOM	334	O	ASN	74	45.384	36.714	17.318	1.00	62.15	A	O
ATOM	335	N	ASN	75	43.597	35.390	17.647	1.00	58.67	A	N
ATOM	336	CA	ASN	75	42.888	35.886	16.481	1.00	55.82	A	C
ATOM	337	CB	ASN	75	42.023	34.785	15.871	1.00	57.81	A	C
ATOM	338	CG	ASN	75	41.410	33.887	16.916	1.00	58.63	A	C
ATOM	339	OD1	ASN	75	40.857	34.358	17.909	1.00	59.69	A	O
ATOM	340	ND2	ASN	75	41.500	32.580	16.697	1.00	58.92	A	N
ATOM	341	C	ASN	75	42.017	37.045	16.918	1.00	52.82	A	C
ATOM	342	O	ASN	75	41.630	37.135	18.081	1.00	53.60	A	O

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(Continued)

## FIG. 4 - 8

ATOM	343	N	ILE	76	41.715	37.937	15.985	1.00	49.11	A	N
ATOM	344	CA	ILE	76	40.893	39.091	16.294	1.00	44.67	A	C
ATOM	345	CB	ILE	76	41.343	40.317	15.502	1.00	44.26	A	C
ATOM	346	CG2	ILE	76	40.565	41.533	15.956	1.00	43.37	A	C
ATOM	347	CG1	ILE	76	42.841	40.547	15.716	1.00	45.27	A	C
ATOM	348	CD1	ILE	76	43.435	41.647	14.844	1.00	45.53	A	C
ATOM	349	C	ILE	76	39.446	38.786	15.964	1.00	42.80	A	C
ATOM	350	O	ILE	76	39.127	38.322	14.868	1.00	41.85	A	O
ATOM	351	N	LEU	77	38.574	39.045	16.930	1.00	40.36	A	N
ATOM	352	CA	LEU	77	37.151	38.801	16.772	1.00	37.65	A	C
ATOM	353	CB	LEU	77	36.636	37.948	17.933	1.00	36.65	A	C
ATOM	354	CG	LEU	77	37.363	36.642	18.264	1.00	35.22	A	C
ATOM	355	CD1	LEU	77	36.600	35.926	19.361	1.00	34.43	A	C
ATOM	356	CD2	LEU	77	37.459	35.756	17.039	1.00	34.38	A	C
ATOM	357	C	LEU	77	36.365	40.107	16.730	1.00	35.91	A	C
ATOM	358	O	LEU	77	36.801	41.123	17.269	1.00	35.03	A	O
ATOM	359	N	VAL	78	35.212	40.069	16.070	1.00	34.19	A	N
ATOM	360	CA	VAL	78	34.330	41.226	15.981	1.00	31.96	A	C
ATOM	361	CB	VAL	78	34.078	41.628	14.509	1.00	31.90	A	C
ATOM	362	CG1	VAL	78	33.612	40.420	13.704	1.00	31.34	A	C
ATOM	363	CG2	VAL	78	33.048	42.747	14.442	1.00	31.56	A	C
ATOM	364	C	VAL	78	33.011	40.838	16.667	1.00	31.15	A	C
ATOM	365	O	VAL	78	32.404	39.819	16.336	1.00	30.46	A	O
ATOM	366	N	PHE	79	32.582	41.643	17.636	1.00	29.90	A	N
ATOM	367	CA	PHE	79	31.358	41.357	18.379	1.00	28.93	A	C
ATOM	368	CB	PHE	79	31.618	41.420	19.888	1.00	29.14	A	C
ATOM	369	CG	PHE	79	32.357	40.238	20.440	1.00	28.39	A	C
ATOM	370	CD1	PHE	79	33.704	40.051	20.165	1.00	28.20	A	C
ATOM	371	CD2	PHE	79	31.701	39.314	21.243	1.00	27.22	A	C
ATOM	372	CE1	PHE	79	34.391	38.956	20.684	1.00	28.13	A	C
ATOM	373	CE2	PHE	79	32.374	38.219	21.764	1.00	27.53	A	C
ATOM	374	CZ	PHE	79	33.725	38.040	21.483	1.00	27.59	A	C
ATOM	375	C	PHE	79	30.186	42.281	18.091	1.00	29.06	A	C
ATOM	376	O	PHE	79	30.354	43.487	17.912	1.00	28.29	A	O
ATOM	377	N	ASN	80	28.990	41.704	18.058	1.00	27.80	A	N
ATOM	378	CA	ASN	80	27.791	42.499	17.864	1.00	27.95	A	C
ATOM	379	CB	ASN	80	26.681	41.670	17.209	1.00	27.03	A	C
ATOM	380	CG	ASN	80	25.354	42.412	17.160	1.00	27.26	A	C
ATOM	381	OD1	ASN	80	24.679	42.587	18.182	1.00	26.87	A	O
ATOM	382	ND2	ASN	80	24.980	42.866	15.974	1.00	26.94	A	N
ATOM	383	C	ASN	80	27.405	42.874	19.289	1.00	28.06	A	C
ATOM	384	O	ASN	80	26.991	42.024	20.066	1.00	28.61	A	O
ATOM	385	N	ALA	81	27.566	44.140	19.642	1.00	28.12	A	N
ATOM	386	CA	ALA	81	27.250	44.579	20.991	1.00	29.16	A	C
ATOM	387	CB	ALA	81	27.503	46.075	21.119	1.00	27.93	A	C
ATOM	388	C	ALA	81	25.818	44.254	21.413	1.00	31.04	A	C
ATOM	389	O	ALA	81	25.582	43.769	22.527	1.00	30.16	A	O
ATOM	390	N	GLU	82	24.870	44.506	20.516	1.00	32.39	A	N
ATOM	391	CA	GLU	82	23.461	44.282	20.809	1.00	34.46	A	C

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(Continued)

## FIG. 4 - 9

ATOM	392	CB	GLU	82	22.602	44.794	19.655	1.00	36.97	A	C
ATOM	393	CG	GLU	82	21.115	44.827	19.968	1.00	40.49	A	C
ATOM	394	CD	GLU	82	20.313	45.538	18.894	1.00	44.05	A	C
ATOM	395	OE1	GLU	82	20.343	45.087	17.726	1.00	45.13	A	O
ATOM	396	OE2	GLU	82	19.652	46.551	19.220	1.00	45.61	A	O
ATOM	397	C	GLU	82	23.042	42.853	21.153	1.00	33.95	A	C
ATOM	398	O	GLU	82	22.055	42.662	21.864	1.00	32.29	A	O
ATOM	399	N	TYR	83	23.777	41.857	20.666	1.00	33.23	A	N
ATOM	400	CA	TYR	83	23.423	40.468	20.947	1.00	33.39	A	C
ATOM	401	CB	TYR	83	22.846	39.810	19.686	1.00	34.54	A	C
ATOM	402	CG	TYR	83	21.690	40.594	19.109	1.00	34.80	A	C
ATOM	403	CD1	TYR	83	20.558	40.859	19.878	1.00	35.22	A	C
ATOM	404	CE1	TYR	83	19.527	41.657	19.396	1.00	36.27	A	C
ATOM	405	CD2	TYR	83	21.759	41.139	17.828	1.00	35.71	A	C
ATOM	406	CE2	TYR	83	20.731	41.940	17.331	1.00	37.42	A	C
ATOM	407	CZ	TYR	83	19.619	42.200	18.125	1.00	37.70	A	C
ATOM	408	OH	TYR	83	18.624	43.044	17.675	1.00	37.69	A	O
ATOM	409	C	TYR	83	24.582	39.644	21.494	1.00	33.19	A	C
ATOM	410	O	TYR	83	24.396	38.511	21.934	1.00	32.91	A	O
ATOM	411	N	GLY	84	25.777	40.217	21.476	1.00	33.53	A	N
ATOM	412	CA	GLY	84	26.933	39.513	21.995	1.00	33.40	A	C
ATOM	413	C	GLY	84	27.454	38.395	21.114	1.00	33.92	A	C
ATOM	414	O	GLY	84	28.329	37.639	21.530	1.00	33.21	A	O
ATOM	415	N	ASN	85	26.918	38.269	19.904	1.00	35.26	A	N
ATOM	416	CA	ASN	85	27.388	37.233	18.993	1.00	37.43	A	C
ATOM	417	CB	ASN	85	26.258	36.780	18.072	1.00	38.34	A	C
ATOM	418	CG	ASN	85	25.764	37.878	17.166	1.00	40.02	A	C
ATOM	419	OD1	ASN	85	25.694	39.040	17.561	1.00	39.96	A	O
ATOM	420	ND2	ASN	85	25.394	37.496	15.950	1.00	41.91	A	N
ATOM	421	C	ASN	85	28.556	37.794	18.188	1.00	38.80	A	C
ATOM	422	O	ASN	85	28.687	39.011	18.035	1.00	40.05	A	O
ATOM	423	N	SER	86	29.410	36.920	17.670	1.00	39.14	A	N
ATOM	424	CA	SER	86	30.565	37.393	16.926	1.00	39.30	A	C
ATOM	425	CB	SER	86	31.723	37.587	17.895	1.00	38.90	A	C
ATOM	426	OG	SER	86	32.041	36.356	18.515	1.00	35.77	A	O
ATOM	427	C	SER	86	31.023	36.482	15.798	1.00	39.94	A	C
ATOM	428	O	SER	86	30.287	35.622	15.323	1.00	41.15	A	O
ATOM	429	N	SER	87	32.264	36.701	15.382	1.00	40.59	A	N
ATOM	430	CA	SER	87	32.916	35.929	14.333	1.00	40.98	A	C
ATOM	431	CB	SER	87	32.152	36.053	13.010	1.00	39.16	A	C
ATOM	432	OG	SER	87	31.727	37.376	12.789	1.00	39.90	A	O
ATOM	433	C	SER	87	34.353	36.433	14.194	1.00	41.10	A	C
ATOM	434	O	SER	87	34.691	37.517	14.682	1.00	41.07	A	O
ATOM	435	N	VAL	88	35.206	35.646	13.548	1.00	41.07	A	N
ATOM	436	CA	VAL	88	36.596	36.043	13.402	1.00	41.43	A	C
ATOM	437	CB	VAL	88	37.502	34.836	13.114	1.00	41.29	A	C
ATOM	438	CG1	VAL	88	38.949	35.295	13.013	1.00	41.30	A	C
ATOM	439	CG2	VAL	88	37.361	33.808	14.222	1.00	40.28	A	C
ATOM	440	C	VAL	88	36.827	37.096	12.331	1.00	41.63	A	C

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(Continued)

## FIG. 4 - 10

ATOM	441	O	VAL	88	36.548	36.885	11.154	1.00	41.38	A	O
ATOM	442	N	PHE	89	37.343	38.238	12.767	1.00	42.23	A	N
ATOM	443	CA	PHE	89	37.641	39.347	11.880	1.00	42.51	A	C
ATOM	444	CB	PHE	89	37.769	40.637	12.699	1.00	40.84	A	C
ATOM	445	CG	PHE	89	37.990	41.865	11.870	1.00	39.96	A	C
ATOM	446	CD1	PHE	89	39.217	42.103	11.265	1.00	39.62	A	C
ATOM	447	CD2	PHE	89	36.963	42.778	11.678	1.00	40.08	A	C
ATOM	448	CE1	PHE	89	39.415	43.231	10.480	1.00	39.60	A	C
ATOM	449	CE2	PHE	89	37.154	43.911	10.894	1.00	39.87	A	C
ATOM	450	CZ	PHE	89	38.381	44.135	10.295	1.00	39.50	A	C
ATOM	451	C	PHE	89	38.956	39.021	11.186	1.00	43.57	A	C
ATOM	452	O	PHE	89	39.156	39.335	10.019	1.00	43.51	A	O
ATOM	453	N	LEU	90	39.851	38.376	11.921	1.00	45.92	A	N
ATOM	454	CA	LEU	90	41.143	38.001	11.380	1.00	48.60	A	C
ATOM	455	CB	LEU	90	42.071	39.213	11.366	1.00	48.66	A	C
ATOM	456	CG	LEU	90	43.033	39.305	10.184	1.00	49.47	A	C
ATOM	457	CD1	LEU	90	42.236	39.408	8.889	1.00	50.17	A	C
ATOM	458	CD2	LEU	90	43.933	40.515	10.346	1.00	49.94	A	C
ATOM	459	C	LEU	90	41.718	36.907	12.267	1.00	50.84	A	C
ATOM	460	O	LEU	90	42.063	37.159	13.421	1.00	50.91	A	O
ATOM	461	N	GLU	91	41.815	35.694	11.726	1.00	53.65	A	N
ATOM	462	CA	GLU	91	42.335	34.559	12.482	1.00	56.17	A	C
ATOM	463	CB	GLU	91	41.817	33.243	11.891	1.00	58.45	A	C
ATOM	464	CG	GLU	91	42.048	33.070	10.403	1.00	60.92	A	C
ATOM	465	CD	GLU	91	41.454	31.774	9.879	1.00	62.39	A	C
ATOM	466	OE1	GLU	91	41.875	30.694	10.350	1.00	63.50	A	O
ATOM	467	OE2	GLU	91	40.566	31.833	9.001	1.00	63.04	A	O
ATOM	468	C	GLU	91	43.855	34.521	12.588	1.00	56.96	A	C
ATOM	469	O	GLU	91	44.572	34.841	11.641	1.00	56.93	A	O
ATOM	470	N	ASN	92	44.322	34.117	13.766	1.00	57.64	A	N
ATOM	471	CA	ASN	92	45.738	34.028	14.100	1.00	58.91	A	C
ATOM	472	CB	ASN	92	45.881	33.389	15.477	1.00	59.59	A	C
ATOM	473	CG	ASN	92	45.129	32.082	15.585	1.00	59.68	A	C
ATOM	474	OD1	ASN	92	45.189	31.248	14.684	1.00	59.97	A	O
ATOM	475	ND2	ASN	92	44.420	31.894	16.691	1.00	61.11	A	N
ATOM	476	C	ASN	92	46.622	33.271	13.111	1.00	59.58	A	C
ATOM	477	O	ASN	92	47.806	33.061	13.370	1.00	59.03	A	O
ATOM	478	N	SER	93	46.059	32.862	11.984	1.00	60.45	A	N
ATOM	479	CA	SER	93	46.828	32.127	10.991	1.00	61.76	A	C
ATOM	480	CB	SER	93	45.978	30.985	10.427	1.00	62.43	A	C
ATOM	481	OG	SER	93	46.714	30.198	9.507	1.00	64.10	A	O
ATOM	482	C	SER	93	47.296	33.030	9.853	1.00	62.23	A	C
ATOM	483	O	SER	93	48.314	32.765	9.213	1.00	62.82	A	O
ATOM	484	N	THR	94	46.552	34.103	9.618	1.00	62.37	A	N
ATOM	485	CA	THR	94	46.852	35.036	8.541	1.00	62.69	A	C
ATOM	486	CB	THR	94	45.982	36.298	8.659	1.00	63.25	A	C
ATOM	487	OG1	THR	94	46.469	37.302	7.759	1.00	63.59	A	O
ATOM	488	CG2	THR	94	46.003	36.821	10.080	1.00	64.14	A	C
ATOM	489	C	THR	94	48.306	35.464	8.377	1.00	62.28	A	C

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(Continued)

## FIG. 4 - 1 1

ATOM	490	O	THR	94	48.882	35.295	7.303	1.00	61.92	A	O
ATOM	491	N	PHE	95	48.908	36.013	9.426	1.00	62.57	A	N
ATOM	492	CA	PHE	95	50.290	36.473	9.322	1.00	63.04	A	C
ATOM	493	CB	PHE	95	50.414	37.889	9.897	1.00	61.98	A	C
ATOM	494	CG	PHE	95	49.456	38.869	9.289	1.00	61.01	A	C
ATOM	495	CD1	PHE	95	48.248	39.155	9.911	1.00	60.97	A	C
ATOM	496	CD2	PHE	95	49.742	39.473	8.073	1.00	60.73	A	C
ATOM	497	CE1	PHE	95	47.337	40.026	9.330	1.00	60.46	A	C
ATOM	498	CE2	PHE	95	48.838	40.343	7.483	1.00	60.09	A	C
ATOM	499	CZ	PHE	95	47.633	40.621	8.113	1.00	61.07	A	C
ATOM	500	C	PHE	95	51.346	35.571	9.956	1.00	63.20	A	C
ATOM	501	O	PHE	95	52.178	36.035	10.736	1.00	63.66	A	O
ATOM	502	N	ASP	96	51.323	34.288	9.611	1.00	63.37	A	N
ATOM	503	CA	ASP	96	52.298	33.347	10.149	1.00	64.05	A	C
ATOM	504	CB	ASP	96	51.771	31.913	10.044	1.00	65.11	A	C
ATOM	505	CG	ASP	96	50.747	31.589	11.115	1.00	65.73	A	C
ATOM	506	OD1	ASP	96	49.758	32.342	11.240	1.00	66.41	A	O
ATOM	507	OD2	ASP	96	50.929	30.580	11.829	1.00	65.32	A	O
ATOM	508	C	ASP	96	53.621	33.470	9.399	1.00	63.82	A	C
ATOM	509	O	ASP	96	54.696	33.433	10.001	1.00	64.05	A	O
ATOM	510	N	GLU	97	53.540	33.619	8.083	1.00	62.95	A	N
ATOM	511	CA	GLU	97	54.740	33.754	7.271	1.00	62.73	A	C
ATOM	512	CB	GLU	97	54.596	32.964	5.965	1.00	65.91	A	C
ATOM	513	CG	GLU	97	54.954	31.478	6.064	1.00	68.84	A	C
ATOM	514	CD	GLU	97	53.945	30.657	6.850	1.00	70.64	A	C
ATOM	515	OE1	GLU	97	54.160	29.432	6.988	1.00	71.38	A	O
ATOM	516	OE2	GLU	97	52.939	31.228	7.325	1.00	71.80	A	O
ATOM	517	C	GLU	97	55.039	35.220	6.963	1.00	60.82	A	C
ATOM	518	O	GLU	97	55.462	35.557	5.857	1.00	60.31	A	O
ATOM	519	N	PHE	98	54.818	36.084	7.952	1.00	58.68	A	N
ATOM	520	CA	PHE	98	55.067	37.513	7.797	1.00	55.93	A	C
ATOM	521	CB	PHE	98	54.200	38.319	8.765	1.00	55.47	A	C
ATOM	522	CG	PHE	98	54.272	39.801	8.542	1.00	54.84	A	C
ATOM	523	CD1	PHE	98	53.712	40.372	7.404	1.00	53.07	A	C
ATOM	524	CD2	PHE	98	54.931	40.624	9.450	1.00	53.89	A	C
ATOM	525	CE1	PHE	98	53.808	41.743	7.173	1.00	53.28	A	C
ATOM	526	CE2	PHE	98	55.032	41.997	9.226	1.00	53.18	A	C
ATOM	527	CZ	PHE	98	54.470	42.556	8.087	1.00	52.22	A	C
ATOM	528	C	PHE	98	56.536	37.820	8.060	1.00	54.61	A	C
ATOM	529	O	PHE	98	57.041	38.878	7.686	1.00	53.80	A	O
ATOM	530	N	GLY	99	57.215	36.885	8.713	1.00	53.53	A	N
ATOM	531	CA	GLY	99	58.624	37.061	9.004	1.00	52.08	A	C
ATOM	532	C	GLY	99	58.908	38.188	9.972	1.00	51.18	A	C
ATOM	533	O	GLY	99	60.037	38.673	10.051	1.00	51.30	A	O
ATOM	534	N	HIS	100	57.884	38.607	10.706	1.00	50.21	A	N
ATOM	535	CA	HIS	100	58.026	39.681	11.686	1.00	49.15	A	C
ATOM	536	CB	HIS	100	57.810	41.049	11.028	1.00	48.84	A	C
ATOM	537	CG	HIS	100	58.850	41.410	10.014	1.00	49.22	A	C
ATOM	538	CD2	HIS	100	58.759	41.613	8.679	1.00	49.42	A	C

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(Continued)

## F I G. 4 - 1 2

ATOM	539	ND1	HIS	100	60.170	41.627	10.346	1.00	49.70	A	N
ATOM	540	CE1	HIS	100	60.848	41.951	9.259	1.00	49.10	A	C
ATOM	541	NE2	HIS	100	60.015	41.949	8.234	1.00	50.14	A	N
ATOM	542	C	HIS	100	57.011	39.511	12.810	1.00	48.06	A	C
ATOM	543	O	HIS	100	55.920	38.977	12.602	1.00	47.18	A	O
ATOM	544	N	SER	101	57.377	39.958	14.005	1.00	46.66	A	N
ATOM	545	CA	SER	101	56.467	39.878	15.136	1.00	45.88	A	C
ATOM	546	CB	SER	101	57.247	39.802	16.446	1.00	47.41	A	C
ATOM	547	OG	SER	101	58.118	38.685	16.447	1.00	51.04	A	O
ATOM	548	C	SER	101	55.617	41.142	15.112	1.00	44.53	A	C
ATOM	549	O	SER	101	56.133	42.248	15.282	1.00	44.41	A	O
ATOM	550	N	ILE	102	54.319	40.976	14.877	1.00	41.90	A	N
ATOM	551	CA	ILE	102	53.409	42.109	14.833	1.00	38.95	A	C
ATOM	552	CB	ILE	102	52.106	41.732	14.117	1.00	38.54	A	C
ATOM	553	CG2	ILE	102	51.153	42.926	14.103	1.00	38.18	A	C
ATOM	554	CG1	ILE	102	52.424	41.288	12.686	1.00	37.65	A	C
ATOM	555	CD1	ILE	102	51.243	40.733	11.937	1.00	37.11	A	C
ATOM	556	C	ILE	102	53.104	42.597	16.244	1.00	38.00	A	C
ATOM	557	O	ILE	102	52.441	41.919	17.024	1.00	38.06	A	O
ATOM	558	N	ASN	103	53.601	43.787	16.556	1.00	37.54	A	N
ATOM	559	CA	ASN	103	53.429	44.399	17.867	1.00	36.65	A	C
ATOM	560	CB	ASN	103	54.437	45.530	18.039	1.00	37.69	A	C
ATOM	561	CG	ASN	103	54.219	46.308	19.315	1.00	39.56	A	C
ATOM	562	OD1	ASN	103	54.655	45.891	20.388	1.00	43.00	A	O
ATOM	563	ND2	ASN	103	53.528	47.439	19.211	1.00	38.34	A	N
ATOM	564	C	ASN	103	52.031	44.953	18.116	1.00	35.79	A	C
ATOM	565	O	ASN	103	51.532	44.910	19.237	1.00	35.79	A	O
ATOM	566	N	ASP	104	51.405	45.490	17.078	1.00	34.43	A	N
ATOM	567	CA	ASP	104	50.079	46.067	17.236	1.00	33.27	A	C
ATOM	568	CB	ASP	104	50.200	47.388	17.998	1.00	34.38	A	C
ATOM	569	CG	ASP	104	48.896	47.823	18.618	1.00	34.79	A	C
ATOM	570	OD1	ASP	104	48.916	48.699	19.509	1.00	33.92	A	O
ATOM	571	OD2	ASP	104	47.852	47.289	18.207	1.00	36.80	A	O
ATOM	572	C	ASP	104	49.436	46.281	15.865	1.00	32.32	A	C
ATOM	573	O	ASP	104	50.124	46.326	14.850	1.00	32.03	A	O
ATOM	574	N	TYR	105	48.118	46.405	15.834	1.00	31.15	A	N
ATOM	575	CA	TYR	105	47.421	46.580	14.570	1.00	32.24	A	C
ATOM	576	CB	TYR	105	46.672	45.296	14.223	1.00	34.70	A	C
ATOM	577	CG	TYR	105	45.443	45.088	15.072	1.00	37.73	A	C
ATOM	578	CD1	TYR	105	44.220	45.636	14.698	1.00	37.51	A	C
ATOM	579	CE1	TYR	105	43.098	45.510	15.506	1.00	40.43	A	C
ATOM	580	CD2	TYR	105	45.514	44.395	16.284	1.00	39.06	A	C
ATOM	581	CE2	TYR	105	44.393	44.263	17.103	1.00	40.75	A	C
ATOM	582	CZ	TYR	105	43.191	44.829	16.705	1.00	41.19	A	C
ATOM	583	OH	TYR	105	42.088	44.755	17.519	1.00	44.27	A	O
ATOM	584	C	TYR	105	46.441	47.743	14.638	1.00	31.43	A	C
ATOM	585	O	TYR	105	46.133	48.249	15.715	1.00	30.78	A	O
ATOM	586	N	SER	106	45.940	48.152	13.479	1.00	30.16	A	N
ATOM	587	CA	SER	106	45.000	49.261	13.415	1.00	29.23	A	C

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(Continued)

## FIG. 4 - 13

ATOM	588	CB	SER	106	45.762	50.588	13.457	1.00	29.81	A	C
ATOM	589	OG	SER	106	44.924	51.668	13.090	1.00	32.32	A	O
ATOM	590	C	SER	106	44.146	49.187	12.157	1.00	27.65	A	C
ATOM	591	O	SER	106	44.657	49.085	11.051	1.00	28.57	A	O
ATOM	592	N	ILE	107	42.835	49.240	12.331	1.00	28.07	A	N
ATOM	593	CA	ILE	107	41.922	49.171	11.198	1.00	27.70	A	C
ATOM	594	CB	ILE	107	40.648	48.352	11.544	1.00	25.83	A	C
ATOM	595	CG2	ILE	107	39.557	48.620	10.522	1.00	26.35	A	C
ATOM	596	CG1	ILE	107	40.970	46.859	11.551	1.00	25.36	A	C
ATOM	597	CD1	ILE	107	41.980	46.457	12.568	1.00	23.77	A	C
ATOM	598	C	ILE	107	41.502	50.556	10.743	1.00	26.85	A	C
ATOM	599	O	ILE	107	41.178	51.420	11.557	1.00	26.55	A	O
ATOM	600	N	SER	108	41.507	50.757	9.432	1.00	27.57	A	N
ATOM	601	CA	SER	108	41.113	52.035	8.862	1.00	26.94	A	C
ATOM	602	CB	SER	108	41.331	52.033	7.346	1.00	26.30	A	C
ATOM	603	OG	SER	108	40.458	51.119	6.700	1.00	23.63	A	O
ATOM	604	C	SER	108	39.639	52.253	9.169	1.00	27.22	A	C
ATOM	605	O	SER	108	38.857	51.310	9.206	1.00	26.49	A	O
ATOM	606	N	PRO	109	39.241	53.506	9.393	1.00	28.50	A	N
ATOM	607	CD	PRO	109	40.025	54.751	9.302	1.00	29.19	A	C
ATOM	608	CA	PRO	109	37.839	53.794	9.693	1.00	29.39	A	C
ATOM	609	CB	PRO	109	37.745	55.294	9.439	1.00	30.19	A	C
ATOM	610	CG	PRO	109	39.080	55.775	9.899	1.00	28.76	A	C
ATOM	611	C	PRO	109	36.842	52.993	8.852	1.00	29.21	A	C
ATOM	612	O	PRO	109	35.901	52.425	9.391	1.00	30.65	A	O
ATOM	613	N	ASP	110	37.046	52.935	7.540	1.00	29.41	A	N
ATOM	614	CA	ASP	110	36.120	52.202	6.676	1.00	28.98	A	C
ATOM	615	CB	ASP	110	36.241	52.673	5.226	1.00	27.99	A	C
ATOM	616	CG	ASP	110	37.613	52.432	4.648	1.00	27.91	A	C
ATOM	617	OD1	ASP	110	38.226	51.397	4.976	1.00	28.41	A	O
ATOM	618	OD2	ASP	110	38.075	53.274	3.852	1.00	29.14	A	O
ATOM	619	C	ASP	110	36.280	50.685	6.715	1.00	29.06	A	C
ATOM	620	O	ASP	110	35.635	49.971	5.953	1.00	30.84	A	O
ATOM	621	N	GLY	111	37.148	50.196	7.589	1.00	28.25	A	N
ATOM	622	CA	GLY	111	37.349	48.766	7.702	1.00	28.14	A	C
ATOM	623	C	GLY	111	37.890	48.064	6.470	1.00	29.53	A	C
ATOM	624	O	GLY	111	37.856	46.837	6.402	1.00	31.16	A	O
ATOM	625	N	GLN	112	38.405	48.818	5.503	1.00	29.61	A	N
ATOM	626	CA	GLN	112	38.946	48.217	4.287	1.00	29.74	A	C
ATOM	627	CB	GLN	112	38.777	49.171	3.109	1.00	29.94	A	C
ATOM	628	CG	GLN	112	37.336	49.442	2.749	1.00	31.79	A	C
ATOM	629	CD	GLN	112	37.191	50.234	1.465	1.00	33.24	A	C
ATOM	630	OE1	GLN	112	36.075	50.474	1.004	1.00	36.27	A	O
ATOM	631	NE2	GLN	112	38.314	50.644	0.880	1.00	31.73	A	N
ATOM	632	C	GLN	112	40.415	47.813	4.390	1.00	30.31	A	C
ATOM	633	O	GLN	112	40.888	46.971	3.631	1.00	31.75	A	O
ATOM	634	N	PHE	113	41.141	48.418	5.320	1.00	29.82	A	N
ATOM	635	CA	PHE	113	42.551	48.106	5.486	1.00	28.23	A	C
ATOM	636	CB	PHE	113	43.428	49.207	4.900	1.00	24.48	A	C

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(Continued)

## FIG. 4 - 14

ATOM	637	CG	PHE	113	43.193	49.467	3.458	1.00	22.98	A	C
ATOM	638	CD1	PHE	113	42.164	50.301	3.052	1.00	20.83	A	C
ATOM	639	CD2	PHE	113	44.010	48.880	2.496	1.00	23.28	A	C
ATOM	640	CE1	PHE	113	41.950	50.552	1.709	1.00	20.79	A	C
ATOM	641	CE2	PHE	113	43.805	49.121	1.150	1.00	22.78	A	C
ATOM	642	CZ	PHE	113	42.771	49.962	0.754	1.00	22.17	A	C
ATOM	643	C	PHE	113	42.919	47.974	6.947	1.00	30.31	A	C
ATOM	644	O	PHE	113	42.234	48.511	7.827	1.00	31.09	A	O
ATOM	645	N	ILE	114	44.013	47.260	7.196	1.00	29.70	A	N
ATOM	646	CA	ILE	114	44.521	47.092	8.542	1.00	30.73	A	C
ATOM	647	CB	ILE	114	44.342	45.642	9.075	1.00	31.72	A	C
ATOM	648	CG2	ILE	114	44.804	44.633	8.042	1.00	33.03	A	C
ATOM	649	CG1	ILE	114	45.128	45.475	10.381	1.00	32.62	A	C
ATOM	650	CD1	ILE	114	45.028	44.092	11.007	1.00	33.60	A	C
ATOM	651	C	ILE	114	46.000	47.457	8.509	1.00	30.59	A	C
ATOM	652	O	ILE	114	46.754	46.974	7.661	1.00	28.76	A	O
ATOM	653	N	LEU	115	46.388	48.343	9.423	1.00	30.68	A	N
ATOM	654	CA	LEU	115	47.759	48.814	9.543	1.00	29.92	A	C
ATOM	655	CB	LEU	115	47.769	50.257	10.053	1.00	30.35	A	C
ATOM	656	CG	LEU	115	49.135	50.941	10.131	1.00	31.72	A	C
ATOM	657	CD1	LEU	115	49.668	51.147	8.718	1.00	33.17	A	C
ATOM	658	CD2	LEU	115	49.018	52.271	10.857	1.00	30.77	A	C
ATOM	659	C	LEU	115	48.481	47.911	10.530	1.00	29.61	A	C
ATOM	660	O	LEU	115	48.127	47.861	11.707	1.00	30.77	A	O
ATOM	661	N	LEU	116	49.484	47.188	10.048	1.00	28.74	A	N
ATOM	662	CA	LEU	116	50.245	46.278	10.891	1.00	28.06	A	C
ATOM	663	CB	LEU	116	50.624	45.023	10.103	1.00	30.07	A	C
ATOM	664	CG	LEU	116	49.450	44.251	9.481	1.00	30.51	A	C
ATOM	665	CD1	LEU	116	49.978	43.171	8.570	1.00	31.10	A	C
ATOM	666	CD2	LEU	116	48.583	43.644	10.573	1.00	30.99	A	C
ATOM	667	C	LEU	116	51.489	46.997	11.363	1.00	28.28	A	C
ATOM	668	O	LEU	116	52.145	47.690	10.591	1.00	30.37	A	O
ATOM	669	N	GLU	117	51.813	46.824	12.634	1.00	27.78	A	N
ATOM	670	CA	GLU	117	52.962	47.484	13.227	1.00	26.58	A	C
ATOM	671	CB	GLU	117	52.476	48.358	14.382	1.00	25.51	A	C
ATOM	672	CG	GLU	117	53.510	49.241	15.036	1.00	23.69	A	C
ATOM	673	CD	GLU	117	52.897	50.076	16.138	1.00	27.72	A	C
ATOM	674	OE1	GLU	117	52.732	49.572	17.268	1.00	29.08	A	O
ATOM	675	OE2	GLU	117	52.552	51.242	15.868	1.00	30.62	A	O
ATOM	676	C	GLU	117	53.997	46.491	13.738	1.00	27.81	A	C
ATOM	677	O	GLU	117	53.666	45.586	14.506	1.00	27.41	A	O
ATOM	678	N	TYR	118	55.247	46.663	13.313	1.00	27.75	A	N
ATOM	679	CA	TYR	118	56.327	45.796	13.765	1.00	29.68	A	C
ATOM	680	CB	TYR	118	56.473	44.586	12.837	1.00	29.52	A	C
ATOM	681	CG	TYR	118	56.819	44.903	11.402	1.00	28.58	A	C
ATOM	682	CD1	TYR	118	55.922	45.572	10.573	1.00	29.31	A	C
ATOM	683	CE1	TYR	118	56.236	45.838	9.239	1.00	28.13	A	C
ATOM	684	CD2	TYR	118	58.040	44.510	10.864	1.00	28.81	A	C
ATOM	685	CE2	TYR	118	58.362	44.769	9.541	1.00	27.91	A	C

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(Continued)

## FIG. 4 - 15

ATOM	686	CZ	TYR	118	57.459	45.431	8.735	1.00	28.04	A	C
ATOM	687	OH	TYR	118	57.792	45.681	7.427	1.00	29.86	A	O
ATOM	688	C	TYR	118	57.641	46.572	13.863	1.00	31.53	A	C
ATOM	689	O	TYR	118	57.683	47.763	13.550	1.00	32.24	A	O
ATOM	690	N	ASN	119	58.708	45.903	14.295	1.00	32.40	A	N
ATOM	691	CA	ASN	119	60.008	46.557	14.459	1.00	33.64	A	C
ATOM	692	CB	ASN	119	60.511	47.128	13.131	1.00	35.42	A	C
ATOM	693	CG	ASN	119	61.069	46.066	12.207	1.00	36.36	A	C
ATOM	694	OD1	ASN	119	61.958	45.306	12.584	1.00	37.66	A	O
ATOM	695	ND2	ASN	119	60.560	46.021	10.983	1.00	37.41	A	N
ATOM	696	C	ASN	119	59.875	47.697	15.464	1.00	34.07	A	C
ATOM	697	O	ASN	119	60.548	48.719	15.348	1.00	34.50	A	O
ATOM	698	N	TYR	120	58.996	47.514	16.443	1.00	33.92	A	N
ATOM	699	CA	TYR	120	58.741	48.517	17.472	1.00	33.38	A	C
ATOM	700	CB	TYR	120	57.510	48.097	18.290	1.00	33.40	A	C
ATOM	701	CG	TYR	120	57.290	48.870	19.569	1.00	33.30	A	C
ATOM	702	CD1	TYR	120	58.029	48.582	20.715	1.00	33.37	A	C
ATOM	703	CE1	TYR	120	57.818	49.284	21.902	1.00	34.88	A	C
ATOM	704	CD2	TYR	120	56.333	49.886	19.636	1.00	33.62	A	C
ATOM	705	CE2	TYR	120	56.114	50.596	20.813	1.00	32.73	A	C
ATOM	706	CZ	TYR	120	56.859	50.289	21.944	1.00	35.24	A	C
ATOM	707	OH	TYR	120	56.643	50.977	23.121	1.00	37.51	A	O
ATOM	708	C	TYR	120	59.933	48.772	18.396	1.00	33.12	A	C
ATOM	709	O	TYR	120	60.472	47.849	19.007	1.00	33.80	A	O
ATOM	710	N	VAL	121	60.330	50.038	18.491	1.00	31.69	A	N
ATOM	711	CA	VAL	121	61.441	50.446	19.343	1.00	30.32	A	C
ATOM	712	CB	VAL	121	62.672	50.845	18.504	1.00	30.75	A	C
ATOM	713	CG1	VAL	121	63.853	51.140	19.420	1.00	28.68	A	C
ATOM	714	CG2	VAL	121	63.013	49.736	17.525	1.00	29.00	A	C
ATOM	715	C	VAL	121	61.008	51.645	20.190	1.00	29.83	A	C
ATOM	716	O	VAL	121	60.788	52.738	19.670	1.00	30.47	A	O
ATOM	717	N	LYS	122	60.889	51.434	21.495	1.00	28.18	A	N
ATOM	718	CA	LYS	122	60.464	52.488	22.404	1.00	27.02	A	C
ATOM	719	CB	LYS	122	60.214	51.910	23.799	1.00	23.73	A	C
ATOM	720	CG	LYS	122	59.793	52.954	24.819	1.00	21.38	A	C
ATOM	721	CD	LYS	122	59.573	52.354	26.191	1.00	20.47	A	C
ATOM	722	CE	LYS	122	59.078	53.406	27.174	1.00	19.23	A	C
ATOM	723	NZ	LYS	122	60.062	54.510	27.346	1.00	18.20	A	N
ATOM	724	C	LYS	122	61.460	53.635	22.528	1.00	27.64	A	C
ATOM	725	O	LYS	122	62.658	53.464	22.315	1.00	28.10	A	O
ATOM	726	N	GLN	123	60.947	54.813	22.860	1.00	27.23	A	N
ATOM	727	CA	GLN	123	61.791	55.979	23.071	1.00	27.82	A	C
ATOM	728	CB	GLN	123	61.607	57.034	21.974	1.00	28.29	A	C
ATOM	729	CG	GLN	123	62.537	58.227	22.164	1.00	28.94	A	C
ATOM	730	CD	GLN	123	62.339	59.308	21.131	1.00	29.91	A	C
ATOM	731	OE1	GLN	123	61.218	59.744	20.889	1.00	32.37	A	O
ATOM	732	NE2	GLN	123	63.431	59.761	20.524	1.00	30.94	A	N
ATOM	733	C	GLN	123	61.385	56.545	24.428	1.00	26.89	A	C
ATOM	734	O	GLN	123	61.837	56.036	25.453	1.00	27.03	A	O

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(Continued)

## FIG. 4 - 16

ATOM	735	N	TRP	124	60.522	57.564	24.444	1.00	23.89	A	N
ATOM	736	CA	TRP	124	60.081	58.149	25.713	1.00	24.21	A	C
ATOM	737	CB	TRP	124	59.886	59.665	25.572	1.00	23.25	A	C
ATOM	738	CG	TRP	124	61.052	60.357	24.934	1.00	19.79	A	C
ATOM	739	CD2	TRP	124	62.444	60.061	25.127	1.00	19.03	A	C
ATOM	740	CE2	TRP	124	63.175	60.913	24.270	1.00	19.13	A	C
ATOM	741	CE3	TRP	124	63.143	59.157	25.936	1.00	15.51	A	C
ATOM	742	CD1	TRP	124	60.999	61.350	24.006	1.00	18.84	A	C
ATOM	743	NE1	TRP	124	62.270	61.690	23.597	1.00	18.74	A	N
ATOM	744	CZ2	TRP	124	64.571	60.885	24.196	1.00	17.77	A	C
ATOM	745	CZ3	TRP	124	64.533	59.129	25.860	1.00	15.41	A	C
ATOM	746	CH2	TRP	124	65.229	59.986	24.996	1.00	17.07	A	C
ATOM	747	C	TRP	124	58.787	57.494	26.209	1.00	24.57	A	C
ATOM	748	O	TRP	124	58.490	56.350	25.861	1.00	25.71	A	O
ATOM	749	N	ARG	125	58.013	58.218	27.013	1.00	24.36	A	N
ATOM	750	CA	ARG	125	56.779	57.670	27.567	1.00	23.36	A	C
ATOM	751	CB	ARG	125	56.189	58.621	28.609	1.00	23.81	A	C
ATOM	752	CG	ARG	125	54.953	58.065	29.308	1.00	23.85	A	C
ATOM	753	CD	ARG	125	54.273	59.129	30.143	1.00	26.24	A	C
ATOM	754	NE	ARG	125	55.090	59.579	31.269	1.00	25.99	A	N
ATOM	755	CZ	ARG	125	55.293	58.867	32.372	1.00	26.04	A	C
ATOM	756	NH1	ARG	125	56.051	59.357	33.347	1.00	24.42	A	N
ATOM	757	NH2	ARG	125	54.735	57.668	32.500	1.00	25.19	A	N
ATOM	758	C	ARG	125	55.706	57.324	26.541	1.00	24.00	A	C
ATOM	759	O	ARG	125	54.935	56.387	26.752	1.00	25.04	A	O
ATOM	760	N	HIS	126	55.651	58.063	25.436	1.00	23.33	A	N
ATOM	761	CA	HIS	126	54.649	57.800	24.403	1.00	22.86	A	C
ATOM	762	CB	HIS	126	53.649	58.943	24.353	1.00	21.14	A	C
ATOM	763	CG	HIS	126	52.987	59.224	25.662	1.00	22.35	A	C
ATOM	764	CD2	HIS	126	53.027	60.316	26.463	1.00	21.51	A	C
ATOM	765	ND1	HIS	126	52.137	58.329	26.274	1.00	22.03	A	N
ATOM	766	CE1	HIS	126	51.679	58.859	27.395	1.00	23.59	A	C
ATOM	767	NE2	HIS	126	52.202	60.064	27.532	1.00	22.48	A	N
ATOM	768	C	HIS	126	55.222	57.599	22.995	1.00	24.43	A	C
ATOM	769	O	HIS	126	54.599	56.947	22.153	1.00	23.99	A	O
ATOM	770	N	SER	127	56.401	58.163	22.744	1.00	23.89	A	N
ATOM	771	CA	SER	127	57.039	58.072	21.434	1.00	24.38	A	C
ATOM	772	CB	SER	127	58.050	59.213	21.267	1.00	23.49	A	C
ATOM	773	OG	SER	127	58.909	59.311	22.387	1.00	23.05	A	O
ATOM	774	C	SER	127	57.737	56.748	21.146	1.00	24.40	A	C
ATOM	775	O	SER	127	58.167	56.050	22.061	1.00	26.55	A	O
ATOM	776	N	TYR	128	57.841	56.420	19.861	1.00	22.67	A	N
ATOM	777	CA	TYR	128	58.501	55.207	19.403	1.00	22.06	A	C
ATOM	778	CB	TYR	128	57.787	53.962	19.928	1.00	21.99	A	C
ATOM	779	CG	TYR	128	56.413	53.712	19.331	1.00	22.49	A	C
ATOM	780	CD1	TYR	128	55.257	54.112	20.003	1.00	23.20	A	C
ATOM	781	CE1	TYR	128	53.992	53.857	19.487	1.00	19.81	A	C
ATOM	782	CD2	TYR	128	56.267	53.049	18.109	1.00	20.70	A	C
ATOM	783	CE2	TYR	128	55.007	52.791	17.580	1.00	20.87	A	C

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(Continued)

## FIG. 4 - 17

ATOM	784	CZ	TYR	128	53.872	53.197	18.279	1.00	22.39	A	C
ATOM	785	OH	TYR	128	52.614	52.946	17.776	1.00	19.88	A	O
ATOM	786	C	TYR	128	58.509	55.160	17.882	1.00	22.84	A	C
ATOM	787	O	TYR	128	57.800	55.922	17.224	1.00	24.63	A	O
ATOM	788	N	THR	129	59.328	54.281	17.320	1.00	22.88	A	N
ATOM	789	CA	THR	129	59.360	54.125	15.874	1.00	25.24	A	C
ATOM	790	CB	THR	129	60.723	54.474	15.245	1.00	27.54	A	C
ATOM	791	OG1	THR	129	61.756	53.676	15.844	1.00	33.01	A	O
ATOM	792	CG2	THR	129	61.025	55.951	15.419	1.00	28.79	A	C
ATOM	793	C	THR	129	59.062	52.675	15.580	1.00	24.85	A	C
ATOM	794	O	THR	129	59.168	51.811	16.457	1.00	22.29	A	O
ATOM	795	N	ALA	130	58.692	52.411	14.337	1.00	24.54	A	N
ATOM	796	CA	ALA	130	58.356	51.062	13.943	1.00	25.98	A	C
ATOM	797	CB	ALA	130	57.061	50.636	14.618	1.00	22.73	A	C
ATOM	798	C	ALA	130	58.195	50.983	12.445	1.00	26.81	A	C
ATOM	799	O	ALA	130	58.277	51.988	11.740	1.00	27.92	A	O
ATOM	800	N	SER	131	57.978	49.767	11.965	1.00	27.15	A	N
ATOM	801	CA	SER	131	57.759	49.540	10.556	1.00	27.62	A	C
ATOM	802	CB	SER	131	58.643	48.403	10.059	1.00	28.58	A	C
ATOM	803	OG	SER	131	59.995	48.822	10.022	1.00	29.90	A	O
ATOM	804	C	SER	131	56.290	49.187	10.426	1.00	27.17	A	C
ATOM	805	O	SER	131	55.651	48.779	11.397	1.00	27.00	A	O
ATOM	806	N	TYR	132	55.747	49.351	9.232	1.00	27.56	A	N
ATOM	807	CA	TYR	132	54.341	49.061	9.029	1.00	28.28	A	C
ATOM	808	CB	TYR	132	53.532	50.357	9.156	1.00	27.16	A	C
ATOM	809	CG	TYR	132	53.649	51.046	10.507	1.00	25.23	A	C
ATOM	810	CD1	TYR	132	52.692	50.842	11.500	1.00	24.00	A	C
ATOM	811	CE1	TYR	132	52.790	51.483	12.735	1.00	23.00	A	C
ATOM	812	CD2	TYR	132	54.714	51.908	10.785	1.00	22.89	A	C
ATOM	813	CE2	TYR	132	54.822	52.549	12.016	1.00	21.43	A	C
ATOM	814	CZ	TYR	132	53.856	52.333	12.985	1.00	22.58	A	C
ATOM	815	OH	TYR	132	53.940	52.976	14.198	1.00	21.69	A	O
ATOM	816	C	TYR	132	54.071	48.418	7.680	1.00	28.72	A	C
ATOM	817	O	TYR	132	54.794	48.639	6.712	1.00	29.54	A	O
ATOM	818	N	ASP	133	53.028	47.604	7.631	1.00	29.99	A	N
ATOM	819	CA	ASP	133	52.629	46.956	6.392	1.00	31.05	A	C
ATOM	820	CB	ASP	133	53.147	45.519	6.314	1.00	31.90	A	C
ATOM	821	CG	ASP	133	54.541	45.436	5.721	1.00	33.92	A	C
ATOM	822	OD1	ASP	133	54.773	46.042	4.649	1.00	33.52	A	O
ATOM	823	OD2	ASP	133	55.400	44.756	6.321	1.00	35.83	A	O
ATOM	824	C	ASP	133	51.125	46.952	6.334	1.00	30.39	A	C
ATOM	825	O	ASP	133	50.467	46.384	7.202	1.00	33.36	A	O
ATOM	826	N	ILE	134	50.579	47.598	5.315	1.00	28.05	A	N
ATOM	827	CA	ILE	134	49.144	47.652	5.157	1.00	25.68	A	C
ATOM	828	CB	ILE	134	48.732	48.816	4.269	1.00	23.81	A	C
ATOM	829	CG2	ILE	134	47.221	48.954	4.289	1.00	22.12	A	C
ATOM	830	CG1	ILE	134	49.421	50.095	4.752	1.00	23.64	A	C
ATOM	831	CD1	ILE	134	49.232	51.277	3.846	1.00	22.40	A	C
ATOM	832	C	ILE	134	48.635	46.368	4.524	1.00	27.46	A	C

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(Continued)

## FIG. 4 - 18

ATOM	833	O	ILE	134	49.171	45.894	3.521	1.00	27.19	A	O
ATOM	834	N	TYR	135	47.599	45.805	5.127	1.00	29.43	A	N
ATOM	835	CA	TYR	135	46.985	44.588	4.628	1.00	30.54	A	C
ATOM	836	CB	TYR	135	46.800	43.588	5.772	1.00	33.25	A	C
ATOM	837	CG	TYR	135	46.276	42.242	5.343	1.00	35.66	A	C
ATOM	838	CD1	TYR	135	47.113	41.311	4.731	1.00	37.89	A	C
ATOM	839	CE1	TYR	135	46.634	40.068	4.319	1.00	40.13	A	C
ATOM	840	CD2	TYR	135	44.939	41.903	5.535	1.00	37.34	A	C
ATOM	841	CE2	TYR	135	44.444	40.666	5.126	1.00	40.17	A	C
ATOM	842	CZ	TYR	135	45.296	39.751	4.518	1.00	41.67	A	C
ATOM	843	OH	TYR	135	44.811	38.526	4.105	1.00	42.54	A	O
ATOM	844	C	TYR	135	45.629	44.990	4.057	1.00	30.05	A	C
ATOM	845	O	TYR	135	44.870	45.705	4.704	1.00	28.31	A	O
ATOM	846	N	ASP	136	45.341	44.536	2.841	1.00	31.33	A	N
ATOM	847	CA	ASP	136	44.083	44.837	2.168	1.00	33.02	A	C
ATOM	848	CB	ASP	136	44.323	44.857	0.655	1.00	32.51	A	C
ATOM	849	CG	ASP	136	43.057	45.095	-0.146	1.00	33.01	A	C
ATOM	850	OD1	ASP	136	43.115	45.872	-1.121	1.00	31.21	A	O
ATOM	851	OD2	ASP	136	42.009	44.500	0.181	1.00	34.97	A	O
ATOM	852	C	ASP	136	43.019	43.797	2.549	1.00	35.55	A	C
ATOM	853	O	ASP	136	42.822	42.810	1.846	1.00	36.12	A	O
ATOM	854	N	LEU	137	42.341	44.040	3.669	1.00	38.03	A	N
ATOM	855	CA	LEU	137	41.303	43.150	4.192	1.00	40.58	A	C
ATOM	856	CB	LEU	137	40.445	43.892	5.225	1.00	40.10	A	C
ATOM	857	CG	LEU	137	41.160	44.413	6.477	1.00	39.13	A	C
ATOM	858	CD1	LEU	137	40.206	45.257	7.307	1.00	37.54	A	C
ATOM	859	CD2	LEU	137	41.686	43.243	7.286	1.00	38.91	A	C
ATOM	860	C	LEU	137	40.392	42.536	3.134	1.00	42.88	A	C
ATOM	861	O	LEU	137	40.038	41.362	3.225	1.00	43.41	A	O
ATOM	862	N	ASN	138	39.997	43.322	2.141	1.00	45.42	A	N
ATOM	863	CA	ASN	138	39.132	42.796	1.093	1.00	48.50	A	C
ATOM	864	CB	ASN	138	38.537	43.936	0.264	1.00	49.71	A	C
ATOM	865	CG	ASN	138	37.127	44.291	0.697	1.00	50.83	A	C
ATOM	866	OD1	ASN	138	36.873	44.555	1.871	1.00	51.97	A	O
ATOM	867	ND2	ASN	138	36.202	44.296	-0.254	1.00	52.74	A	N
ATOM	868	C	ASN	138	39.884	41.824	0.191	1.00	49.47	A	C
ATOM	869	O	ASN	138	39.642	40.619	0.240	1.00	50.62	A	O
ATOM	870	N	LYS	139	40.794	42.346	-0.626	1.00	50.26	A	N
ATOM	871	CA	LYS	139	41.581	41.507	-1.526	1.00	51.09	A	C
ATOM	872	CB	LYS	139	42.510	42.374	-2.382	1.00	51.15	A	C
ATOM	873	CG	LYS	139	41.785	43.427	-3.212	1.00	53.38	A	C
ATOM	874	CD	LYS	139	42.753	44.331	-3.974	1.00	54.25	A	C
ATOM	875	CE	LYS	139	43.550	43.564	-5.021	1.00	56.31	A	C
ATOM	876	NZ	LYS	139	44.447	44.453	-5.817	1.00	56.39	A	N
ATOM	877	C	LYS	139	42.413	40.528	-0.703	1.00	51.63	A	C
ATOM	878	O	LYS	139	43.148	39.708	-1.251	1.00	51.80	A	O
ATOM	879	N	ARG	140	42.288	40.624	0.618	1.00	51.49	A	N
ATOM	880	CA	ARG	140	43.025	39.768	1.534	1.00	51.71	A	C
ATOM	881	CB	ARG	140	42.338	38.408	1.642	1.00	53.88	A	C

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(Continued)

## FIG. 4 - 19

ATOM	882	CG	ARG	140	40.911	38.495	2.157	1.00	57.36	A	C
ATOM	883	CD	ARG	140	40.257	37.128	2.211	1.00	60.02	A	C
ATOM	884	NE	ARG	140	40.936	36.235	3.142	1.00	62.76	A	N
ATOM	885	CZ	ARG	140	40.633	34.950	3.294	1.00	64.87	A	C
ATOM	886	NH1	ARG	140	39.661	34.409	2.570	1.00	66.83	A	N
ATOM	887	NH2	ARG	140	41.298	34.206	4.169	1.00	65.62	A	N
ATOM	888	C	ARG	140	44.464	39.603	1.066	1.00	50.29	A	C
ATOM	889	O	ARG	140	44.992	38.496	1.002	1.00	50.21	A	O
ATOM	890	N	GLN	141	45.096	40.723	0.741	1.00	49.82	A	N
ATOM	891	CA	GLN	141	46.473	40.707	0.268	1.00	48.70	A	C
ATOM	892	CB	GLN	141	46.487	40.815	-1.260	1.00	50.32	A	C
ATOM	893	CG	GLN	141	47.774	40.348	-1.909	1.00	55.02	A	C
ATOM	894	CD	GLN	141	47.640	40.179	-3.413	1.00	57.33	A	C
ATOM	895	OE1	GLN	141	48.582	39.756	-4.088	1.00	57.97	A	O
ATOM	896	NE2	GLN	141	46.465	40.509	-3.947	1.00	58.85	A	N
ATOM	897	C	GLN	141	47.293	41.837	0.898	1.00	46.02	A	C
ATOM	898	O	GLN	141	46.761	42.880	1.274	1.00	45.33	A	O
ATOM	899	N	LEU	142	48.594	41.610	1.013	1.00	43.34	A	N
ATOM	900	CA	LEU	142	49.505	42.578	1.605	1.00	41.50	A	C
ATOM	901	CB	LEU	142	50.638	41.824	2.296	1.00	41.17	A	C
ATOM	902	CG	LEU	142	51.489	42.501	3.359	1.00	42.33	A	C
ATOM	903	CD1	LEU	142	52.443	41.463	3.922	1.00	42.24	A	C
ATOM	904	CD2	LEU	142	52.254	43.677	2.772	1.00	42.66	A	C
ATOM	905	C	LEU	142	50.062	43.498	0.520	1.00	40.87	A	C
ATOM	906	O	LEU	142	50.557	43.030	-0.506	1.00	41.57	A	O
ATOM	907	N	ILE	143	49.978	44.806	0.748	1.00	39.20	A	N
ATOM	908	CA	ILE	143	50.466	45.789	-0.217	1.00	37.17	A	C
ATOM	909	CB	ILE	143	49.921	47.202	0.104	1.00	36.58	A	C
ATOM	910	CG2	ILE	143	50.486	48.225	-0.874	1.00	35.56	A	C
ATOM	911	CG1	ILE	143	48.398	47.197	0.030	1.00	34.64	A	C
ATOM	912	CD1	ILE	143	47.777	48.494	0.468	1.00	37.28	A	C
ATOM	913	C	ILE	143	51.985	45.843	-0.209	1.00	36.06	A	C
ATOM	914	O	ILE	143	52.603	45.859	0.849	1.00	36.63	A	O
ATOM	915	N	THR	144	52.592	45.882	-1.386	1.00	35.40	A	N
ATOM	916	CA	THR	144	54.046	45.933	-1.459	1.00	35.79	A	C
ATOM	917	CB	THR	144	54.616	44.654	-2.124	1.00	35.59	A	C
ATOM	918	OG1	THR	144	54.192	44.592	-3.491	1.00	37.13	A	O
ATOM	919	CG2	THR	144	54.121	43.415	-1.403	1.00	33.21	A	C
ATOM	920	C	THR	144	54.515	47.152	-2.243	1.00	35.43	A	C
ATOM	921	O	THR	144	55.700	47.311	-2.511	1.00	36.45	A	O
ATOM	922	N	GLU	145	53.577	48.015	-2.602	1.00	36.27	A	N
ATOM	923	CA	GLU	145	53.891	49.214	-3.369	1.00	36.32	A	C
ATOM	924	CB	GLU	145	52.962	49.297	-4.586	1.00	38.36	A	C
ATOM	925	CG	GLU	145	53.553	48.748	-5.875	1.00	42.66	A	C
ATOM	926	CD	GLU	145	54.667	49.639	-6.418	1.00	45.91	A	C
ATOM	927	OE1	GLU	145	55.745	49.705	-5.779	1.00	45.49	A	O
ATOM	928	OE2	GLU	145	54.456	50.283	-7.476	1.00	45.56	A	O
ATOM	929	C	GLU	145	53.775	50.496	-2.544	1.00	35.06	A	C
ATOM	930	O	GLU	145	52.874	50.635	-1.715	1.00	34.22	A	O

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(Continued)

## FIG. 4 - 20

ATOM	931	N	GLU	146	54.692	51.428	-2.782	1.00	33.82	A	N
ATOM	932	CA	GLU	146	54.699	52.706	-2.079	1.00	32.54	A	C
ATOM	933	CB	GLU	146	53.594	53.608	-2.630	1.00	33.84	A	C
ATOM	934	CG	GLU	146	53.708	53.924	-4.107	1.00	33.18	A	C
ATOM	935	CD	GLU	146	54.992	54.651	-4.455	1.00	33.14	A	C
ATOM	936	OE1	GLU	146	55.677	55.129	-3.528	1.00	32.11	A	O
ATOM	937	OE2	GLU	146	55.309	54.754	-5.660	1.00	35.19	A	O
ATOM	938	C	GLU	146	54.495	52.521	-0.579	1.00	32.26	A	C
ATOM	939	O	GLU	146	53.644	53.172	0.031	1.00	32.38	A	O
ATOM	940	N	ARG	147	55.287	51.638	0.013	1.00	30.84	A	N
ATOM	941	CA	ARG	147	55.185	51.357	1.437	1.00	29.94	A	C
ATOM	942	CB	ARG	147	55.992	50.107	1.774	1.00	31.91	A	C
ATOM	943	CG	ARG	147	55.376	48.821	1.262	1.00	33.35	A	C
ATOM	944	CD	ARG	147	55.999	47.649	1.963	1.00	34.66	A	C
ATOM	945	NE	ARG	147	57.415	47.539	1.650	1.00	37.64	A	N
ATOM	946	CZ	ARG	147	58.271	46.812	2.356	1.00	39.76	A	C
ATOM	947	NH1	ARG	147	57.844	46.143	3.421	1.00	40.68	A	N
ATOM	948	NH2	ARG	147	59.546	46.737	1.987	1.00	39.79	A	N
ATOM	949	C	ARG	147	55.623	52.483	2.363	1.00	28.99	A	C
ATOM	950	O	ARG	147	56.440	53.330	2.002	1.00	29.74	A	O
ATOM	951	N	ILE	148	55.066	52.486	3.568	1.00	26.79	A	N
ATOM	952	CA	ILE	148	55.430	53.484	4.555	1.00	25.21	A	C
ATOM	953	CB	ILE	148	54.537	53.364	5.798	1.00	24.62	A	C
ATOM	954	CG2	ILE	148	55.096	54.201	6.940	1.00	25.09	A	C
ATOM	955	CG1	ILE	148	53.116	53.794	5.427	1.00	23.14	A	C
ATOM	956	CD1	ILE	148	52.107	53.642	6.533	1.00	23.82	A	C
ATOM	957	C	ILE	148	56.879	53.173	4.891	1.00	24.99	A	C
ATOM	958	O	ILE	148	57.240	52.014	5.068	1.00	26.06	A	O
ATOM	959	N	PRO	149	57.735	54.201	4.974	1.00	24.98	A	N
ATOM	960	CD	PRO	149	57.443	55.645	4.930	1.00	24.87	A	C
ATOM	961	CA	PRO	149	59.148	53.966	5.282	1.00	26.52	A	C
ATOM	962	CB	PRO	149	59.765	55.356	5.151	1.00	24.90	A	C
ATOM	963	CG	PRO	149	58.659	56.244	5.614	1.00	24.49	A	C
ATOM	964	C	PRO	149	59.421	53.352	6.642	1.00	27.89	A	C
ATOM	965	O	PRO	149	58.621	53.489	7.567	1.00	27.47	A	O
ATOM	966	N	ASN	150	60.551	52.657	6.748	1.00	29.59	A	N
ATOM	967	CA	ASN	150	60.950	52.064	8.016	1.00	30.82	A	C
ATOM	968	CB	ASN	150	62.154	51.131	7.830	1.00	32.43	A	C
ATOM	969	CG	ASN	150	61.775	49.805	7.189	1.00	35.16	A	C
ATOM	970	OD1	ASN	150	60.749	49.215	7.530	1.00	36.40	A	O
ATOM	971	ND2	ASN	150	62.612	49.319	6.271	1.00	36.52	A	N
ATOM	972	C	ASN	150	61.336	53.245	8.900	1.00	30.50	A	C
ATOM	973	O	ASN	150	61.583	54.348	8.394	1.00	31.20	A	O
ATOM	974	N	ASN	151	61.387	53.022	10.208	1.00	28.46	A	N
ATOM	975	CA	ASN	151	61.734	54.078	11.154	1.00	28.87	A	C
ATOM	976	CB	ASN	151	63.137	54.622	10.877	1.00	30.74	A	C
ATOM	977	CG	ASN	151	64.213	53.571	11.048	1.00	34.06	A	C
ATOM	978	OD1	ASN	151	64.360	52.678	10.219	1.00	36.24	A	O
ATOM	979	ND2	ASN	151	64.965	53.666	12.139	1.00	37.62	A	N

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(Continued)

## FIG. 4 - 2 1

ATOM	980	C	ASN	151	60.734	55.230	11.111	1.00	28.16	A	C
ATOM	981	O	ASN	151	61.118	56.400	11.112	1.00	28.85	A	O
ATOM	982	N	THR	152	59.450	54.895	11.064	1.00	26.20	A	N
ATOM	983	CA	THR	152	58.415	55.911	11.041	1.00	24.74	A	C
ATOM	984	CB	THR	152	57.119	55.389	10.399	1.00	25.27	A	C
ATOM	985	OG1	THR	152	57.351	55.125	9.009	1.00	24.18	A	O
ATOM	986	CG2	THR	152	56.004	56.426	10.538	1.00	23.99	A	C
ATOM	987	C	THR	152	58.139	56.319	12.474	1.00	23.46	A	C
ATOM	988	O	THR	152	57.933	55.476	13.340	1.00	25.16	A	O
ATOM	989	N	GLN	153	58.134	57.620	12.721	1.00	22.30	A	N
ATOM	990	CA	GLN	153	57.916	58.129	14.063	1.00	20.67	A	C
ATOM	991	CB	GLN	153	58.501	59.534	14.161	1.00	19.09	A	C
ATOM	992	CG	GLN	153	60.002	59.543	13.906	1.00	13.74	A	C
ATOM	993	CD	GLN	153	60.495	60.853	13.331	1.00	14.57	A	C
ATOM	994	OE1	GLN	153	60.089	61.260	12.233	1.00	12.70	A	O
ATOM	995	NE2	GLN	153	61.375	61.524	14.066	1.00	10.81	A	N
ATOM	996	C	GLN	153	56.460	58.112	14.495	1.00	20.53	A	C
ATOM	997	O	GLN	153	56.163	57.979	15.683	1.00	19.36	A	O
ATOM	998	N	TRP	154	55.556	58.229	13.531	1.00	20.90	A	N
ATOM	999	CA	TRP	154	54.131	58.213	13.831	1.00	21.02	A	C
ATOM	1000	CB	TRP	154	53.733	59.498	14.550	1.00	22.43	A	C
ATOM	1001	CG	TRP	154	52.312	59.530	14.923	1.00	21.90	A	C
ATOM	1002	CD2	TRP	154	51.695	58.791	15.976	1.00	22.22	A	C
ATOM	1003	CE2	TRP	154	50.315	59.087	15.942	1.00	23.62	A	C
ATOM	1004	CE3	TRP	154	52.173	57.902	16.947	1.00	22.95	A	C
ATOM	1005	CD1	TRP	154	51.321	60.228	14.308	1.00	24.44	A	C
ATOM	1006	NE1	TRP	154	50.112	59.968	14.912	1.00	24.78	A	N
ATOM	1007	CZ2	TRP	154	49.404	58.526	16.842	1.00	22.94	A	C
ATOM	1008	CZ3	TRP	154	51.263	57.339	17.847	1.00	22.07	A	C
ATOM	1009	CH2	TRP	154	49.897	57.656	17.784	1.00	23.43	A	C
ATOM	1010	C	TRP	154	53.291	58.054	12.576	1.00	21.43	A	C
ATOM	1011	O	TRP	154	53.642	58.572	11.518	1.00	22.33	A	O
ATOM	1012	N	VAL	155	52.173	57.343	12.703	1.00	21.97	A	N
ATOM	1013	CA	VAL	155	51.267	57.103	11.579	1.00	20.81	A	C
ATOM	1014	CB	VAL	155	51.642	55.797	10.840	1.00	19.96	A	C
ATOM	1015	CG1	VAL	155	51.835	54.687	11.842	1.00	21.34	A	C
ATOM	1016	CG2	VAL	155	50.562	55.414	9.833	1.00	20.23	A	C
ATOM	1017	C	VAL	155	49.840	57.004	12.104	1.00	21.39	A	C
ATOM	1018	O	VAL	155	49.601	56.425	13.162	1.00	21.74	A	O
ATOM	1019	N	THR	156	48.898	57.576	11.364	1.00	20.70	A	N
ATOM	1020	CA	THR	156	47.504	57.557	11.768	1.00	21.67	A	C
ATOM	1021	CB	THR	156	47.189	58.736	12.716	1.00	22.79	A	C
ATOM	1022	OG1	THR	156	45.771	58.848	12.890	1.00	25.50	A	O
ATOM	1023	CG2	THR	156	47.707	60.031	12.145	1.00	22.46	A	C
ATOM	1024	C	THR	156	46.558	57.633	10.577	1.00	22.20	A	C
ATOM	1025	O	THR	156	46.861	58.276	9.577	1.00	22.72	A	O
ATOM	1026	N	TRP	157	45.413	56.966	10.689	1.00	21.38	A	N
ATOM	1027	CA	TRP	157	44.423	56.985	9.627	1.00	21.45	A	C
ATOM	1028	CB	TRP	157	43.426	55.825	9.765	1.00	21.88	A	C

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(Continued)

## FIG. 4 - 22

ATOM	1029	CG	TRP	157	43.995	54.450	9.599	1.00	20.88	A	C
ATOM	1030	CD2	TRP	157	44.315	53.800	8.364	1.00	18.96	A	C
ATOM	1031	CE2	TRP	157	44.843	52.531	8.686	1.00	19.67	A	C
ATOM	1032	CE3	TRP	157	44.208	54.168	7.019	1.00	17.93	A	C
ATOM	1033	CD1	TRP	157	44.328	53.571	10.592	1.00	20.82	A	C
ATOM	1034	NE1	TRP	157	44.838	52.417	10.052	1.00	21.01	A	N
ATOM	1035	CZ2	TRP	157	45.265	51.626	7.708	1.00	19.12	A	C
ATOM	1036	CZ3	TRP	157	44.627	53.267	6.046	1.00	19.76	A	C
ATOM	1037	CH2	TRP	157	45.149	52.011	6.397	1.00	19.30	A	C
ATOM	1038	C	TRP	157	43.650	58.276	9.801	1.00	23.03	A	C
ATOM	1039	O	TRP	157	43.750	58.917	10.843	1.00	25.03	A	O
ATOM	1040	N	SER	158	42.889	58.663	8.784	1.00	23.17	A	N
ATOM	1041	CA	SER	158	42.064	59.855	8.889	1.00	23.44	A	C
ATOM	1042	CB	SER	158	41.667	60.362	7.502	1.00	22.82	A	C
ATOM	1043	OG	SER	158	41.208	59.311	6.679	1.00	23.84	A	O
ATOM	1044	C	SER	158	40.845	59.377	9.678	1.00	23.86	A	C
ATOM	1045	O	SER	158	40.613	58.176	9.781	1.00	24.35	A	O
ATOM	1046	N	PRO	159	40.056	60.301	10.247	1.00	24.17	A	N
ATOM	1047	CD	PRO	159	40.136	61.762	10.114	1.00	24.24	A	C
ATOM	1048	CA	PRO	159	38.876	59.922	11.029	1.00	23.40	A	C
ATOM	1049	CB	PRO	159	38.270	61.264	11.419	1.00	23.45	A	C
ATOM	1050	CG	PRO	159	39.427	62.214	11.353	1.00	24.19	A	C
ATOM	1051	C	PRO	159	37.901	59.090	10.224	1.00	25.36	A	C
ATOM	1052	O	PRO	159	37.191	58.248	10.771	1.00	27.14	A	O
ATOM	1053	N	VAL	160	37.878	59.334	8.919	1.00	25.28	A	N
ATOM	1054	CA	VAL	160	36.977	58.640	8.014	1.00	23.99	A	C
ATOM	1055	CB	VAL	160	35.784	59.545	7.689	1.00	24.54	A	C
ATOM	1056	CG1	VAL	160	35.066	59.064	6.449	1.00	26.50	A	C
ATOM	1057	CG2	VAL	160	34.834	59.559	8.875	1.00	26.15	A	C
ATOM	1058	C	VAL	160	37.679	58.218	6.730	1.00	23.78	A	C
ATOM	1059	O	VAL	160	38.570	58.908	6.245	1.00	24.51	A	O
ATOM	1060	N	GLY	161	37.268	57.080	6.181	1.00	24.05	A	N
ATOM	1061	CA	GLY	161	37.876	56.579	4.962	1.00	22.93	A	C
ATOM	1062	C	GLY	161	39.121	55.786	5.286	1.00	23.87	A	C
ATOM	1063	O	GLY	161	39.144	55.045	6.269	1.00	24.24	A	O
ATOM	1064	N	HIS	162	40.164	55.950	4.476	1.00	25.01	A	N
ATOM	1065	CA	HIS	162	41.423	55.239	4.695	1.00	25.86	A	C
ATOM	1066	CB	HIS	162	41.419	53.923	3.920	1.00	26.04	A	C
ATOM	1067	CG	HIS	162	41.075	54.087	2.475	1.00	27.52	A	C
ATOM	1068	CD2	HIS	162	41.614	54.875	1.515	1.00	27.58	A	C
ATOM	1069	ND1	HIS	162	40.039	53.402	1.874	1.00	27.77	A	N
ATOM	1070	CE1	HIS	162	39.956	53.764	0.606	1.00	28.51	A	C
ATOM	1071	NE2	HIS	162	40.900	54.656	0.363	1.00	28.82	A	N
ATOM	1072	C	HIS	162	42.660	56.053	4.305	1.00	25.44	A	C
ATOM	1073	O	HIS	162	43.636	55.501	3.794	1.00	24.38	A	O
ATOM	1074	N	LYS	163	42.609	57.364	4.527	1.00	24.47	A	N
ATOM	1075	CA	LYS	163	43.751	58.221	4.224	1.00	23.45	A	C
ATOM	1076	CB	LYS	163	43.372	59.701	4.273	1.00	21.75	A	C
ATOM	1077	CG	LYS	163	42.528	60.216	3.130	1.00	21.55	A	C

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(Continued)

## FIG. 4 - 23

ATOM	1078	CD	LYS	163	42.281	61.706	3.335	1.00	20.23	A	C
ATOM	1079	CE	LYS	163	41.464	62.316	2.228	1.00	18.07	A	C
ATOM	1080	NZ	LYS	163	41.315	63.778	2.422	1.00	20.95	A	N
ATOM	1081	C	LYS	163	44.781	57.961	5.309	1.00	23.44	A	C
ATOM	1082	O	LYS	163	44.425	57.600	6.433	1.00	23.42	A	O
ATOM	1083	N	LEU	164	46.053	58.146	4.979	1.00	23.11	A	N
ATOM	1084	CA	LEU	164	47.117	57.937	5.950	1.00	23.65	A	C
ATOM	1085	CB	LEU	164	48.014	56.773	5.524	1.00	24.35	A	C
ATOM	1086	CG	LEU	164	47.551	55.351	5.848	1.00	25.57	A	C
ATOM	1087	CD1	LEU	164	48.519	54.349	5.219	1.00	25.59	A	C
ATOM	1088	CD2	LEU	164	47.497	55.162	7.359	1.00	25.62	A	C
ATOM	1089	C	LEU	164	47.970	59.182	6.120	1.00	23.21	A	C
ATOM	1090	O	LEU	164	48.175	59.943	5.177	1.00	24.34	A	O
ATOM	1091	N	ALA	165	48.456	59.383	7.335	1.00	21.88	A	N
ATOM	1092	CA	ALA	165	49.319	60.508	7.649	1.00	21.58	A	C
ATOM	1093	CB	ALA	165	48.548	61.583	8.376	1.00	21.77	A	C
ATOM	1094	C	ALA	165	50.406	59.953	8.545	1.00	22.07	A	C
ATOM	1095	O	ALA	165	50.115	59.285	9.537	1.00	22.91	A	O
ATOM	1096	N	TYR	166	51.661	60.208	8.201	1.00	22.02	A	N
ATOM	1097	CA	TYR	166	52.745	59.697	9.024	1.00	21.73	A	C
ATOM	1098	CB	TYR	166	53.185	58.319	8.520	1.00	22.38	A	C
ATOM	1099	CG	TYR	166	53.814	58.315	7.141	1.00	22.11	A	C
ATOM	1100	CD1	TYR	166	55.148	58.661	6.964	1.00	21.28	A	C
ATOM	1101	CE1	TYR	166	55.733	58.638	5.704	1.00	22.05	A	C
ATOM	1102	CD2	TYR	166	53.074	57.949	6.015	1.00	20.67	A	C
ATOM	1103	CE2	TYR	166	53.648	57.923	4.753	1.00	20.02	A	C
ATOM	1104	CZ	TYR	166	54.981	58.268	4.603	1.00	21.75	A	C
ATOM	1105	OH	TYR	166	55.566	58.252	3.352	1.00	20.77	A	O
ATOM	1106	C	TYR	166	53.927	60.643	9.057	1.00	21.64	A	C
ATOM	1107	O	TYR	166	54.108	61.464	8.157	1.00	21.61	A	O
ATOM	1108	N	VAL	167	54.722	60.529	10.111	1.00	20.28	A	N
ATOM	1109	CA	VAL	167	55.886	61.371	10.264	1.00	19.16	A	C
ATOM	1110	CB	VAL	167	55.924	62.011	11.644	1.00	19.56	A	C
ATOM	1111	CG1	VAL	167	57.103	62.984	11.731	1.00	18.58	A	C
ATOM	1112	CG2	VAL	167	54.609	62.713	11.916	1.00	18.36	A	C
ATOM	1113	C	VAL	167	57.135	60.537	10.078	1.00	20.06	A	C
ATOM	1114	O	VAL	167	57.287	59.474	10.679	1.00	21.80	A	O
ATOM	1115	N	TRP	168	58.030	61.023	9.233	1.00	19.65	A	N
ATOM	1116	CA	TRP	168	59.268	60.320	8.964	1.00	19.61	A	C
ATOM	1117	CB	TRP	168	59.164	59.558	7.646	1.00	20.07	A	C
ATOM	1118	CG	TRP	168	60.387	58.772	7.353	1.00	23.12	A	C
ATOM	1119	CD2	TRP	168	61.319	59.011	6.300	1.00	21.38	A	C
ATOM	1120	CE2	TRP	168	62.353	58.061	6.436	1.00	21.58	A	C
ATOM	1121	CE3	TRP	168	61.382	59.936	5.256	1.00	21.74	A	C
ATOM	1122	CD1	TRP	168	60.873	57.712	8.066	1.00	22.86	A	C
ATOM	1123	NE1	TRP	168	62.056	57.281	7.521	1.00	21.54	A	N
ATOM	1124	CZ2	TRP	168	63.445	58.012	5.563	1.00	23.71	A	C
ATOM	1125	CZ3	TRP	168	62.468	59.889	4.386	1.00	23.21	A	C
ATOM	1126	CH2	TRP	168	63.484	58.934	4.546	1.00	22.74	A	C

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(Continued)

## FIG. 4 - 24

ATOM	1127	C	TRP	168	60.406	61.327	8.906	1.00	19.17	A	C
ATOM	1128	O	TRP	168	60.331	62.319	8.187	1.00	19.01	A	O
ATOM	1129	N	ASN	169	61.452	61.072	9.682	1.00	19.26	A	N
ATOM	1130	CA	ASN	169	62.589	61.969	9.732	1.00	21.05	A	C
ATOM	1131	CB	ASN	169	63.374	61.902	8.417	1.00	23.39	A	C
ATOM	1132	CG	ASN	169	64.056	60.565	8.217	1.00	26.24	A	C
ATOM	1133	OD1	ASN	169	64.410	60.196	7.097	1.00	29.51	A	O
ATOM	1134	ND2	ASN	169	64.255	59.832	9.307	1.00	27.22	A	N
ATOM	1135	C	ASN	169	62.122	63.394	10.007	1.00	19.72	A	C
ATOM	1136	O	ASN	169	62.582	64.344	9.378	1.00	19.61	A	O
ATOM	1137	N	ASN	170	61.182	63.522	10.938	1.00	19.01	A	N
ATOM	1138	CA	ASN	170	60.654	64.817	11.354	1.00	18.95	A	C
ATOM	1139	CB	ASN	170	61.806	65.679	11.887	1.00	19.76	A	C
ATOM	1140	CG	ASN	170	62.326	65.193	13.239	1.00	21.23	A	C
ATOM	1141	OD1	ASN	170	62.690	64.025	13.404	1.00	23.29	A	O
ATOM	1142	ND2	ASN	170	62.362	66.092	14.210	1.00	21.16	A	N
ATOM	1143	C	ASN	170	59.828	65.621	10.341	1.00	18.94	A	C
ATOM	1144	O	ASN	170	59.594	66.815	10.541	1.00	17.99	A	O
ATOM	1145	N	ASP	171	59.385	64.974	9.264	1.00	18.46	A	N
ATOM	1146	CA	ASP	171	58.566	65.643	8.254	1.00	18.64	A	C
ATOM	1147	CB	ASP	171	59.271	65.696	6.898	1.00	18.52	A	C
ATOM	1148	CG	ASP	171	60.353	66.750	6.836	1.00	17.77	A	C
ATOM	1149	OD1	ASP	171	60.126	67.876	7.307	1.00	17.30	A	O
ATOM	1150	OD2	ASP	171	61.436	66.454	6.294	1.00	24.17	A	O
ATOM	1151	C	ASP	171	57.255	64.888	8.099	1.00	20.36	A	C
ATOM	1152	O	ASP	171	57.182	63.690	8.382	1.00	21.44	A	O
ATOM	1153	N	ILE	172	56.225	65.585	7.632	1.00	19.52	A	N
ATOM	1154	CA	ILE	172	54.908	64.983	7.466	1.00	18.52	A	C
ATOM	1155	CB	ILE	172	53.813	65.966	7.899	1.00	18.99	A	C
ATOM	1156	CG2	ILE	172	52.443	65.329	7.734	1.00	17.69	A	C
ATOM	1157	CG1	ILE	172	54.053	66.394	9.350	1.00	18.78	A	C
ATOM	1158	CD1	ILE	172	53.167	67.538	9.795	1.00	18.44	A	C
ATOM	1159	C	ILE	172	54.609	64.539	6.044	1.00	18.52	A	C
ATOM	1160	O	ILE	172	54.905	65.246	5.085	1.00	19.61	A	O
ATOM	1161	N	TYR	173	54.017	63.358	5.921	1.00	17.61	A	N
ATOM	1162	CA	TYR	173	53.645	62.808	4.625	1.00	16.59	A	C
ATOM	1163	CB	TYR	173	54.519	61.612	4.256	1.00	14.94	A	C
ATOM	1164	CG	TYR	173	55.983	61.921	4.121	1.00	15.66	A	C
ATOM	1165	CD1	TYR	173	56.815	61.978	5.237	1.00	16.67	A	C
ATOM	1166	CE1	TYR	173	58.170	62.271	5.100	1.00	16.34	A	C
ATOM	1167	CD2	TYR	173	56.541	62.165	2.870	1.00	15.99	A	C
ATOM	1168	CE2	TYR	173	57.879	62.460	2.727	1.00	13.89	A	C
ATOM	1169	CZ	TYR	173	58.685	62.512	3.838	1.00	15.53	A	C
ATOM	1170	OH	TYR	173	60.004	62.837	3.678	1.00	21.66	A	O
ATOM	1171	C	TYR	173	52.198	62.341	4.679	1.00	17.34	A	C
ATOM	1172	O	TYR	173	51.683	62.008	5.748	1.00	14.56	A	O
ATOM	1173	N	VAL	174	51.552	62.306	3.518	1.00	18.18	A	N
ATOM	1174	CA	VAL	174	50.174	61.865	3.444	1.00	19.46	A	C
ATOM	1175	CB	VAL	174	49.212	63.060	3.319	1.00	18.88	A	C

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(Continued)

## FIG. 4 - 25

ATOM	1176	CG1	VAL	174	47.775	62.564	3.207	1.00	19.37	A	C
ATOM	1177	CG2	VAL	174	49.359	63.969	4.534	1.00	20.44	A	C
ATOM	1178	C	VAL	174	49.948	60.928	2.268	1.00	21.57	A	C
ATOM	1179	O	VAL	174	50.485	61.129	1.185	1.00	22.86	A	O
ATOM	1180	N	LYS	175	49.154	59.891	2.500	1.00	23.19	A	N
ATOM	1181	CA	LYS	175	48.824	58.934	1.461	1.00	23.86	A	C
ATOM	1182	CB	LYS	175	49.275	57.516	1.831	1.00	24.28	A	C
ATOM	1183	CG	LYS	175	50.759	57.352	2.113	1.00	28.82	A	C
ATOM	1184	CD	LYS	175	51.100	55.895	2.422	1.00	29.18	A	C
ATOM	1185	CE	LYS	175	51.107	55.043	1.163	1.00	29.84	A	C
ATOM	1186	NZ	LYS	175	52.263	55.409	0.291	1.00	31.80	A	N
ATOM	1187	C	LYS	175	47.314	58.935	1.338	1.00	24.49	A	C
ATOM	1188	O	LYS	175	46.615	58.606	2.293	1.00	25.05	A	O
ATOM	1189	N	ILE	176	46.820	59.319	0.166	1.00	24.77	A	N
ATOM	1190	CA	ILE	176	45.394	59.327	-0.102	1.00	24.70	A	C
ATOM	1191	CB	ILE	176	45.095	60.028	-1.437	1.00	22.88	A	C
ATOM	1192	CG2	ILE	176	43.605	60.073	-1.679	1.00	21.75	A	C
ATOM	1193	CG1	ILE	176	45.677	61.443	-1.423	1.00	21.52	A	C
ATOM	1194	CD1	ILE	176	45.016	62.379	-0.424	1.00	23.58	A	C
ATOM	1195	C	ILE	176	44.995	57.860	-0.211	1.00	26.89	A	C
ATOM	1196	O	ILE	176	43.979	57.428	0.328	1.00	26.38	A	O
ATOM	1197	N	GLU	177	45.829	57.097	-0.906	1.00	29.47	A	N
ATOM	1198	CA	GLU	177	45.597	55.672	-1.104	1.00	31.88	A	C
ATOM	1199	CB	GLU	177	45.412	55.380	-2.594	1.00	35.29	A	C
ATOM	1200	CG	GLU	177	44.308	56.190	-3.248	1.00	38.36	A	C
ATOM	1201	CD	GLU	177	42.925	55.776	-2.784	1.00	41.13	A	C
ATOM	1202	OE1	GLU	177	41.951	56.495	-3.105	1.00	45.06	A	O
ATOM	1203	OE2	GLU	177	42.810	54.730	-2.107	1.00	40.42	A	O
ATOM	1204	C	GLU	177	46.796	54.895	-0.569	1.00	31.55	A	C
ATOM	1205	O	GLU	177	47.940	55.223	-0.872	1.00	31.59	A	O
ATOM	1206	N	PRO	178	46.544	53.840	0.221	1.00	31.40	A	N
ATOM	1207	CD	PRO	178	45.218	53.240	0.438	1.00	30.50	A	C
ATOM	1208	CA	PRO	178	47.591	53.000	0.814	1.00	29.97	A	C
ATOM	1209	CB	PRO	178	46.796	51.902	1.509	1.00	30.05	A	C
ATOM	1210	CG	PRO	178	45.567	51.805	0.684	1.00	31.07	A	C
ATOM	1211	C	PRO	178	48.633	52.436	-0.150	1.00	29.50	A	C
ATOM	1212	O	PRO	178	49.727	52.062	0.269	1.00	31.00	A	O
ATOM	1213	N	ASN	179	48.308	52.379	-1.436	1.00	28.20	A	N
ATOM	1214	CA	ASN	179	49.251	51.838	-2.409	1.00	27.53	A	C
ATOM	1215	CB	ASN	179	48.568	50.805	-3.299	1.00	26.23	A	C
ATOM	1216	CG	ASN	179	47.474	51.409	-4.144	1.00	25.74	A	C
ATOM	1217	OD1	ASN	179	46.494	51.948	-3.626	1.00	26.59	A	O
ATOM	1218	ND2	ASN	179	47.635	51.329	-5.452	1.00	26.72	A	N
ATOM	1219	C	ASN	179	49.854	52.916	-3.285	1.00	27.48	A	C
ATOM	1220	O	ASN	179	50.818	52.670	-4.004	1.00	28.42	A	O
ATOM	1221	N	LEU	180	49.289	54.115	-3.231	1.00	26.68	A	N
ATOM	1222	CA	LEU	180	49.805	55.200	-4.050	1.00	26.11	A	C
ATOM	1223	CB	LEU	180	48.658	56.125	-4.456	1.00	24.86	A	C
ATOM	1224	CG	LEU	180	47.574	55.370	-5.238	1.00	25.87	A	C

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(Continued)

## FIG. 4 - 26

ATOM	1225	CD1	LEU	180	46.604	56.359	-5.856	1.00	23.58	A	C
ATOM	1226	CD2	LEU	180	48.224	54.503	-6.328	1.00	22.86	A	C
ATOM	1227	C	LEU	180	50.938	55.996	-3.391	1.00	25.78	A	C
ATOM	1228	O	LEU	180	51.185	55.883	-2.185	1.00	23.62	A	O
ATOM	1229	N	PRO	181	51.669	56.789	-4.194	1.00	24.96	A	N
ATOM	1230	CD	PRO	181	51.687	56.842	-5.667	1.00	23.41	A	C
ATOM	1231	CA	PRO	181	52.766	57.580	-3.634	1.00	23.35	A	C
ATOM	1232	CB	PRO	181	53.403	58.217	-4.870	1.00	22.16	A	C
ATOM	1233	CG	PRO	181	53.124	57.201	-5.944	1.00	22.72	A	C
ATOM	1234	C	PRO	181	52.216	58.613	-2.667	1.00	22.15	A	C
ATOM	1235	O	PRO	181	51.144	59.173	-2.880	1.00	21.88	A	O
ATOM	1236	N	SER	182	52.954	58.864	-1.601	1.00	21.65	A	N
ATOM	1237	CA	SER	182	52.516	59.829	-0.620	1.00	20.50	A	C
ATOM	1238	CB	SER	182	52.999	59.404	0.765	1.00	22.61	A	C
ATOM	1239	OG	SER	182	54.408	59.345	0.806	1.00	23.55	A	O
ATOM	1240	C	SER	182	53.034	61.222	-0.947	1.00	19.05	A	C
ATOM	1241	O	SER	182	54.003	61.380	-1.687	1.00	17.74	A	O
ATOM	1242	N	TYR	183	52.366	62.233	-0.402	1.00	17.87	A	N
ATOM	1243	CA	TYR	183	52.786	63.606	-0.611	1.00	15.17	A	C
ATOM	1244	CB	TYR	183	51.595	64.523	-0.832	1.00	12.09	A	C
ATOM	1245	CG	TYR	183	50.676	64.028	-1.905	1.00	12.54	A	C
ATOM	1246	CD1	TYR	183	49.729	63.052	-1.625	1.00	8.93	A	C
ATOM	1247	CE1	TYR	183	48.916	62.554	-2.610	1.00	11.95	A	C
ATOM	1248	CD2	TYR	183	50.782	64.494	-3.214	1.00	9.42	A	C
ATOM	1249	CE2	TYR	183	49.961	63.990	-4.218	1.00	10.27	A	C
ATOM	1250	CZ	TYR	183	49.032	63.019	-3.903	1.00	10.59	A	C
ATOM	1251	OH	TYR	183	48.205	62.494	-4.867	1.00	14.71	A	O
ATOM	1252	C	TYR	183	53.532	64.067	0.617	1.00	15.72	A	C
ATOM	1253	O	TYR	183	53.208	63.679	1.740	1.00	17.69	A	O
ATOM	1254	N	ARG	184	54.540	64.893	0.386	1.00	14.64	A	N
ATOM	1255	CA	ARG	184	55.342	65.436	1.452	1.00	14.10	A	C
ATOM	1256	CB	ARG	184	56.786	65.593	0.970	1.00	16.84	A	C
ATOM	1257	CG	ARG	184	57.725	66.203	1.989	1.00	20.48	A	C
ATOM	1258	CD	ARG	184	59.170	65.912	1.629	1.00	20.61	A	C
ATOM	1259	NE	ARG	184	60.095	66.485	2.598	1.00	20.21	A	N
ATOM	1260	CZ	ARG	184	61.407	66.288	2.583	1.00	19.46	A	C
ATOM	1261	NH1	ARG	184	61.954	65.529	1.650	1.00	17.13	A	N
ATOM	1262	NH2	ARG	184	62.170	66.853	3.506	1.00	20.35	A	N
ATOM	1263	C	ARG	184	54.736	66.779	1.820	1.00	14.10	A	C
ATOM	1264	O	ARG	184	54.569	67.650	0.972	1.00	14.71	A	O
ATOM	1265	N	ILE	185	54.390	66.937	3.089	1.00	15.27	A	N
ATOM	1266	CA	ILE	185	53.804	68.175	3.572	1.00	14.44	A	C
ATOM	1267	CB	ILE	185	52.786	67.884	4.692	1.00	16.20	A	C
ATOM	1268	CG2	ILE	185	52.091	69.175	5.115	1.00	14.78	A	C
ATOM	1269	CG1	ILE	185	51.770	66.842	4.202	1.00	15.25	A	C
ATOM	1270	CD1	ILE	185	51.021	67.250	2.947	1.00	12.00	A	C
ATOM	1271	C	ILE	185	54.847	69.172	4.091	1.00	14.33	A	C
ATOM	1272	O	ILE	185	54.647	70.377	3.994	1.00	14.95	A	O
ATOM	1273	N	THR	186	55.950	68.676	4.646	1.00	14.38	A	N

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(Continued)

## FIG. 4 - 27

ATOM	1274	CA	THR	186	56.995	69.555	5.169	1.00	15.05	A	C
ATOM	1275	CB	THR	186	57.051	69.549	6.717	1.00	15.72	A	C
ATOM	1276	OG1	THR	186	57.308	68.218	7.181	1.00	18.48	A	O
ATOM	1277	CG2	THR	186	55.734	70.060	7.323	1.00	13.92	A	C
ATOM	1278	C	THR	186	58.384	69.190	4.663	1.00	17.06	A	C
ATOM	1279	O	THR	186	58.643	68.055	4.262	1.00	19.33	A	O
ATOM	1280	N	TRP	187	59.275	70.174	4.696	1.00	18.28	A	N
ATOM	1281	CA	TRP	187	60.655	70.020	4.253	1.00	16.04	A	C
ATOM	1282	CB	TRP	187	60.843	70.734	2.915	1.00	13.96	A	C
ATOM	1283	CG	TRP	187	60.392	69.949	1.736	1.00	14.75	A	C
ATOM	1284	CD2	TRP	187	59.055	69.841	1.234	1.00	15.37	A	C
ATOM	1285	CE2	TRP	187	59.093	68.954	0.135	1.00	15.22	A	C
ATOM	1286	CE3	TRP	187	57.829	70.405	1.606	1.00	12.92	A	C
ATOM	1287	CD1	TRP	187	61.165	69.149	0.941	1.00	14.94	A	C
ATOM	1288	NE1	TRP	187	60.392	68.549	-0.020	1.00	15.60	A	N
ATOM	1289	CZ2	TRP	187	57.949	68.616	-0.597	1.00	17.91	A	C
ATOM	1290	CZ3	TRP	187	56.692	70.074	0.881	1.00	16.75	A	C
ATOM	1291	CH2	TRP	187	56.758	69.185	-0.211	1.00	17.84	A	C
ATOM	1292	C	TRP	187	61.607	70.620	5.292	1.00	15.71	A	C
ATOM	1293	O	TRP	187	62.804	70.725	5.053	1.00	19.54	A	O
ATOM	1294	N	THR	188	61.077	70.999	6.449	1.00	13.19	A	N
ATOM	1295	CA	THR	188	61.892	71.605	7.493	1.00	11.35	A	C
ATOM	1296	CB	THR	188	61.122	72.737	8.180	1.00	11.04	A	C
ATOM	1297	OG1	THR	188	59.835	72.253	8.587	1.00	9.11	A	O
ATOM	1298	CG2	THR	188	60.955	73.920	7.232	1.00	7.35	A	C
ATOM	1299	C	THR	188	62.384	70.642	8.572	1.00	12.10	A	C
ATOM	1300	O	THR	188	63.198	71.016	9.415	1.00	9.49	A	O
ATOM	1301	N	GLY	189	61.881	69.412	8.552	1.00	14.44	A	N
ATOM	1302	CA	GLY	189	62.296	68.426	9.538	1.00	16.08	A	C
ATOM	1303	C	GLY	189	63.794	68.421	9.782	1.00	15.86	A	C
ATOM	1304	O	GLY	189	64.584	68.685	8.881	1.00	17.65	A	O
ATOM	1305	N	LYS	190	64.196	68.117	11.004	1.00	17.28	A	N
ATOM	1306	CA	LYS	190	65.612	68.096	11.346	1.00	18.87	A	C
ATOM	1307	CB	LYS	190	66.189	69.512	11.264	1.00	20.03	A	C
ATOM	1308	CG	LYS	190	67.679	69.588	11.472	1.00	22.58	A	C
ATOM	1309	CD	LYS	190	68.181	70.997	11.256	1.00	27.62	A	C
ATOM	1310	CE	LYS	190	69.698	71.060	11.386	1.00	31.27	A	C
ATOM	1311	NZ	LYS	190	70.207	72.451	11.273	1.00	35.57	A	N
ATOM	1312	C	LYS	190	65.799	67.530	12.747	1.00	18.55	A	C
ATOM	1313	O	LYS	190	65.384	68.134	13.737	1.00	18.41	A	O
ATOM	1314	N	GLU	191	66.426	66.362	12.811	1.00	19.79	A	N
ATOM	1315	CA	GLU	191	66.674	65.661	14.062	1.00	21.70	A	C
ATOM	1316	CB	GLU	191	67.796	64.653	13.851	1.00	23.41	A	C
ATOM	1317	CG	GLU	191	67.894	63.598	14.937	1.00	29.95	A	C
ATOM	1318	CD	GLU	191	69.018	62.605	14.689	1.00	30.89	A	C
ATOM	1319	OE1	GLU	191	68.970	61.497	15.262	1.00	33.70	A	O
ATOM	1320	OE2	GLU	191	69.952	62.932	13.929	1.00	33.21	A	O
ATOM	1321	C	GLU	191	67.015	66.583	15.236	1.00	21.53	A	C
ATOM	1322	O	GLU	191	67.930	67.397	15.156	1.00	22.21	A	O

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(Continued)

## FIG. 4 - 28

ATOM	1323	N	ASP	192	66.262	66.451	16.320	1.00	21.17	A	N
ATOM	1324	CA	ASP	192	66.470	67.246	17.525	1.00	22.27	A	C
ATOM	1325	CB	ASP	192	67.810	66.880	18.182	1.00	23.92	A	C
ATOM	1326	CG	ASP	192	67.922	65.400	18.510	1.00	25.20	A	C
ATOM	1327	OD1	ASP	192	66.891	64.775	18.850	1.00	25.70	A	O
ATOM	1328	OD2	ASP	192	69.049	64.866	18.438	1.00	26.25	A	O
ATOM	1329	C	ASP	192	66.425	68.759	17.341	1.00	21.93	A	C
ATOM	1330	O	ASP	192	66.998	69.489	18.145	1.00	22.78	A	O
ATOM	1331	N	ILE	193	65.748	69.242	16.304	1.00	21.66	A	N
ATOM	1332	CA	ILE	193	65.685	70.684	16.071	1.00	20.08	A	C
ATOM	1333	CB	ILE	193	66.747	71.113	15.039	1.00	20.73	A	C
ATOM	1334	CG2	ILE	193	66.570	72.567	14.677	1.00	18.91	A	C
ATOM	1335	CG1	ILE	193	68.142	70.889	15.624	1.00	22.58	A	C
ATOM	1336	CD1	ILE	193	69.263	71.198	14.671	1.00	26.43	A	C
ATOM	1337	C	ILE	193	64.318	71.172	15.615	1.00	19.15	A	C
ATOM	1338	O	ILE	193	63.736	72.068	16.220	1.00	19.55	A	O
ATOM	1339	N	ILE	194	63.814	70.594	14.534	1.00	19.04	A	N
ATOM	1340	CA	ILE	194	62.506	70.967	14.021	1.00	17.41	A	C
ATOM	1341	CB	ILE	194	62.596	71.547	12.587	1.00	18.89	A	C
ATOM	1342	CG2	ILE	194	61.209	71.944	12.095	1.00	16.97	A	C
ATOM	1343	CG1	ILE	194	63.551	72.750	12.553	1.00	19.26	A	C
ATOM	1344	CD1	ILE	194	63.118	73.936	13.395	1.00	16.78	A	C
ATOM	1345	C	ILE	194	61.663	69.702	13.969	1.00	18.22	A	C
ATOM	1346	O	ILE	194	62.066	68.713	13.349	1.00	17.31	A	O
ATOM	1347	N	TYR	195	60.511	69.726	14.642	1.00	17.31	A	N
ATOM	1348	CA	TYR	195	59.592	68.593	14.639	1.00	16.19	A	C
ATOM	1349	CB	TYR	195	59.338	68.071	16.053	1.00	17.03	A	C
ATOM	1350	CG	TYR	195	60.560	67.776	16.893	1.00	17.58	A	C
ATOM	1351	CD1	TYR	195	61.427	68.802	17.286	1.00	18.28	A	C
ATOM	1352	CE1	TYR	195	62.485	68.558	18.145	1.00	16.45	A	C
ATOM	1353	CD2	TYR	195	60.799	66.490	17.377	1.00	15.00	A	C
ATOM	1354	CE2	TYR	195	61.859	66.237	18.240	1.00	15.14	A	C
ATOM	1355	CZ	TYR	195	62.694	67.275	18.624	1.00	17.41	A	C
ATOM	1356	OH	TYR	195	63.725	67.041	19.515	1.00	21.26	A	O
ATOM	1357	C	TYR	195	58.242	69.016	14.047	1.00	16.29	A	C
ATOM	1358	O	TYR	195	57.574	69.902	14.586	1.00	15.85	A	O
ATOM	1359	N	ASN	196	57.851	68.380	12.942	1.00	15.27	A	N
ATOM	1360	CA	ASN	196	56.578	68.656	12.286	1.00	12.88	A	C
ATOM	1361	CB	ASN	196	56.772	68.894	10.790	1.00	13.47	A	C
ATOM	1362	CG	ASN	196	57.591	70.133	10.489	1.00	14.66	A	C
ATOM	1363	OD1	ASN	196	57.132	71.261	10.678	1.00	10.34	A	O
ATOM	1364	ND2	ASN	196	58.819	69.927	10.013	1.00	15.26	A	N
ATOM	1365	C	ASN	196	55.686	67.438	12.457	1.00	14.12	A	C
ATOM	1366	O	ASN	196	56.050	66.347	12.044	1.00	16.31	A	O
ATOM	1367	N	GLY	197	54.522	67.613	13.065	1.00	14.48	A	N
ATOM	1368	CA	GLY	197	53.622	66.488	13.231	1.00	15.17	A	C
ATOM	1369	C	GLY	197	53.880	65.638	14.458	1.00	15.48	A	C
ATOM	1370	O	GLY	197	53.059	64.799	14.815	1.00	15.55	A	O
ATOM	1371	N	ILE	198	55.023	65.846	15.098	1.00	16.49	A	N

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(Continued)

## FIG. 4 - 29

ATOM	1372	CA	ILE	198	55.378	65.097	16.298	1.00	16.59	A	C
ATOM	1373	CB	ILE	198	56.425	63.991	16.011	1.00	18.21	A	C
ATOM	1374	CG2	ILE	198	55.874	63.013	14.987	1.00	18.51	A	C
ATOM	1375	CG1	ILE	198	57.724	64.602	15.494	1.00	17.86	A	C
ATOM	1376	CD1	ILE	198	58.798	63.565	15.214	1.00	19.35	A	C
ATOM	1377	C	ILE	198	55.946	66.057	17.318	1.00	15.95	A	C
ATOM	1378	O	ILE	198	56.507	67.091	16.966	1.00	17.63	A	O
ATOM	1379	N	THR	199	55.809	65.700	18.583	1.00	15.42	A	N
ATOM	1380	CA	THR	199	56.264	66.547	19.672	1.00	16.68	A	C
ATOM	1381	CB	THR	199	55.374	66.316	20.908	1.00	17.40	A	C
ATOM	1382	OG1	THR	199	55.462	64.944	21.301	1.00	18.82	A	O
ATOM	1383	CG2	THR	199	53.924	66.619	20.583	1.00	15.72	A	C
ATOM	1384	C	THR	199	57.716	66.334	20.076	1.00	16.00	A	C
ATOM	1385	O	THR	199	58.317	65.325	19.734	1.00	16.12	A	O
ATOM	1386	N	ASP	200	58.276	67.301	20.801	1.00	16.87	A	N
ATOM	1387	CA	ASP	200	59.649	67.193	21.289	1.00	15.49	A	C
ATOM	1388	CB	ASP	200	60.315	68.576	21.418	1.00	14.82	A	C
ATOM	1389	CG	ASP	200	59.681	69.446	22.491	1.00	17.16	A	C
ATOM	1390	OD1	ASP	200	58.517	69.190	22.873	1.00	16.41	A	O
ATOM	1391	OD2	ASP	200	60.348	70.403	22.945	1.00	15.97	A	O
ATOM	1392	C	ASP	200	59.496	66.515	22.641	1.00	15.54	A	C
ATOM	1393	O	ASP	200	58.388	66.118	22.999	1.00	17.01	A	O
ATOM	1394	N	TRP	201	60.581	66.381	23.395	1.00	15.10	A	N
ATOM	1395	CA	TRP	201	60.504	65.699	24.672	1.00	13.14	A	C
ATOM	1396	CB	TRP	201	61.885	65.619	25.326	1.00	14.90	A	C
ATOM	1397	CG	TRP	201	61.905	64.679	26.510	1.00	15.25	A	C
ATOM	1398	CD2	TRP	201	61.412	64.953	27.828	1.00	13.65	A	C
ATOM	1399	CE2	TRP	201	61.500	63.753	28.564	1.00	13.52	A	C
ATOM	1400	CE3	TRP	201	60.902	66.096	28.456	1.00	11.78	A	C
ATOM	1401	CD1	TRP	201	62.269	63.360	26.507	1.00	13.81	A	C
ATOM	1402	NE1	TRP	201	62.025	62.799	27.733	1.00	13.64	A	N
ATOM	1403	CZ2	TRP	201	61.096	63.661	29.897	1.00	14.03	A	C
ATOM	1404	CZ3	TRP	201	60.502	66.009	29.778	1.00	12.04	A	C
ATOM	1405	CH2	TRP	201	60.601	64.797	30.486	1.00	14.87	A	C
ATOM	1406	C	TRP	201	59.529	66.327	25.662	1.00	14.42	A	C
ATOM	1407	O	TRP	201	58.635	65.656	26.175	1.00	13.63	A	O
ATOM	1408	N	VAL	202	59.691	67.615	25.931	1.00	15.14	A	N
ATOM	1409	CA	VAL	202	58.830	68.265	26.911	1.00	14.23	A	C
ATOM	1410	CB	VAL	202	59.402	69.639	27.330	1.00	12.99	A	C
ATOM	1411	CG1	VAL	202	59.010	70.716	26.322	1.00	11.02	A	C
ATOM	1412	CG2	VAL	202	58.947	69.963	28.753	1.00	8.71	A	C
ATOM	1413	C	VAL	202	57.365	68.401	26.518	1.00	15.76	A	C
ATOM	1414	O	VAL	202	56.497	68.404	27.391	1.00	18.74	A	O
ATOM	1415	N	TYR	203	57.072	68.518	25.226	1.00	15.58	A	N
ATOM	1416	CA	TYR	203	55.676	68.606	24.805	1.00	14.25	A	C
ATOM	1417	CB	TYR	203	55.556	69.078	23.354	1.00	14.63	A	C
ATOM	1418	CG	TYR	203	55.227	70.542	23.227	1.00	12.35	A	C
ATOM	1419	CD1	TYR	203	56.231	71.508	23.193	1.00	11.91	A	C
ATOM	1420	CE1	TYR	203	55.920	72.867	23.108	1.00	11.20	A	C

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(Continued)

## FIG. 4 - 30

ATOM	1421	CD2	TYR	203	53.902	70.966	23.177	1.00	12.17	A	C
ATOM	1422	CE2	TYR	203	53.579	72.314	23.099	1.00	10.57	A	C
ATOM	1423	CZ	TYR	203	54.588	73.259	23.061	1.00	9.67	A	C
ATOM	1424	OH	TYR	203	54.259	74.586	22.970	1.00	7.05	A	O
ATOM	1425	C	TYR	203	55.024	67.234	24.951	1.00	14.92	A	C
ATOM	1426	O	TYR	203	53.896	67.124	25.406	1.00	15.28	A	O
ATOM	1427	N	GLU	204	55.744	66.185	24.570	1.00	16.35	A	N
ATOM	1428	CA	GLU	204	55.222	64.826	24.684	1.00	16.96	A	C
ATOM	1429	CB	GLU	204	56.238	63.812	24.130	1.00	14.28	A	C
ATOM	1430	CG	GLU	204	55.928	62.380	24.540	1.00	14.97	A	C
ATOM	1431	CD	GLU	204	56.872	61.345	23.947	1.00	19.54	A	C
ATOM	1432	OE1	GLU	204	56.697	60.144	24.271	1.00	18.49	A	O
ATOM	1433	OE2	GLU	204	57.778	61.714	23.160	1.00	18.73	A	O
ATOM	1434	C	GLU	204	54.868	64.431	26.128	1.00	18.02	A	C
ATOM	1435	O	GLU	204	53.816	63.848	26.388	1.00	17.48	A	O
ATOM	1436	N	GLU	205	55.757	64.761	27.059	1.00	18.67	A	N
ATOM	1437	CA	GLU	205	55.589	64.409	28.459	1.00	20.30	A	C
ATOM	1438	CB	GLU	205	56.970	64.250	29.096	1.00	20.92	A	C
ATOM	1439	CG	GLU	205	56.958	64.035	30.592	1.00	24.62	A	C
ATOM	1440	CD	GLU	205	56.563	62.625	30.974	1.00	28.17	A	C
ATOM	1441	OE1	GLU	205	56.398	62.355	32.182	1.00	32.15	A	O
ATOM	1442	OE2	GLU	205	56.424	61.778	30.069	1.00	31.11	A	O
ATOM	1443	C	GLU	205	54.760	65.362	29.319	1.00	22.25	A	C
ATOM	1444	O	GLU	205	53.996	64.915	30.164	1.00	22.34	A	O
ATOM	1445	N	GLU	206	54.902	66.666	29.107	1.00	22.70	A	N
ATOM	1446	CA	GLU	206	54.202	67.632	29.939	1.00	23.19	A	C
ATOM	1447	CB	GLU	206	55.203	68.667	30.453	1.00	25.39	A	C
ATOM	1448	CG	GLU	206	56.466	68.088	31.080	1.00	27.87	A	C
ATOM	1449	CD	GLU	206	56.188	67.307	32.345	1.00	29.45	A	C
ATOM	1450	OE1	GLU	206	57.160	66.855	32.987	1.00	29.92	A	O
ATOM	1451	OE2	GLU	206	55.000	67.144	32.696	1.00	29.12	A	O
ATOM	1452	C	GLU	206	53.024	68.378	29.324	1.00	24.91	A	C
ATOM	1453	O	GLU	206	52.175	68.885	30.051	1.00	24.03	A	O
ATOM	1454	N	VAL	207	52.957	68.452	27.999	1.00	25.41	A	N
ATOM	1455	CA	VAL	207	51.880	69.199	27.375	1.00	25.29	A	C
ATOM	1456	CB	VAL	207	52.444	70.235	26.398	1.00	25.95	A	C
ATOM	1457	CG1	VAL	207	51.324	71.114	25.876	1.00	28.49	A	C
ATOM	1458	CG2	VAL	207	53.496	71.080	27.092	1.00	26.77	A	C
ATOM	1459	C	VAL	207	50.801	68.409	26.653	1.00	26.09	A	C
ATOM	1460	O	VAL	207	49.617	68.703	26.813	1.00	27.62	A	O
ATOM	1461	N	PHE	208	51.194	67.412	25.865	1.00	26.41	A	N
ATOM	1462	CA	PHE	208	50.228	66.620	25.105	1.00	26.03	A	C
ATOM	1463	CB	PHE	208	50.557	66.676	23.607	1.00	27.43	A	C
ATOM	1464	CG	PHE	208	50.234	67.994	22.962	1.00	28.64	A	C
ATOM	1465	CD1	PHE	208	51.234	68.911	22.679	1.00	29.07	A	C
ATOM	1466	CD2	PHE	208	48.918	68.328	22.660	1.00	30.01	A	C
ATOM	1467	CE1	PHE	208	50.929	70.142	22.104	1.00	30.28	A	C
ATOM	1468	CE2	PHE	208	48.604	69.556	22.086	1.00	30.23	A	C
ATOM	1469	CZ	PHE	208	49.612	70.464	21.809	1.00	30.40	A	C

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(Continued)

## FIG. 4 - 31

ATOM	1470	C	PHE	208	50.082	65.163	25.506	1.00	26.13	A	C
ATOM	1471	O	PHE	208	49.215	64.471	24.985	1.00	27.79	A	O
ATOM	1472	N	SER	209	50.918	64.687	26.421	1.00	26.62	A	N
ATOM	1473	CA	SER	209	50.852	63.293	26.848	1.00	25.74	A	C
ATOM	1474	CB	SER	209	49.645	63.059	27.743	1.00	24.80	A	C
ATOM	1475	OG	SER	209	49.871	63.629	29.014	1.00	29.47	A	O
ATOM	1476	C	SER	209	50.773	62.377	25.642	1.00	25.50	A	C
ATOM	1477	O	SER	209	50.278	61.249	25.716	1.00	25.72	A	O
ATOM	1478	N	ALA	210	51.272	62.875	24.524	1.00	23.72	A	N
ATOM	1479	CA	ALA	210	51.263	62.112	23.299	1.00	22.80	A	C
ATOM	1480	CB	ALA	210	49.977	62.364	22.530	1.00	20.62	A	C
ATOM	1481	C	ALA	210	52.455	62.560	22.492	1.00	21.87	A	C
ATOM	1482	O	ALA	210	52.986	63.644	22.703	1.00	22.09	A	O
ATOM	1483	N	TYR	211	52.863	61.719	21.558	1.00	21.57	A	N
ATOM	1484	CA	TYR	211	54.000	62.009	20.718	1.00	21.42	A	C
ATOM	1485	CB	TYR	211	54.725	60.711	20.405	1.00	19.58	A	C
ATOM	1486	CG	TYR	211	55.921	60.870	19.528	1.00	16.81	A	C
ATOM	1487	CD1	TYR	211	56.853	61.870	19.770	1.00	16.07	A	C
ATOM	1488	CE1	TYR	211	58.002	61.971	19.001	1.00	18.18	A	C
ATOM	1489	CD2	TYR	211	56.160	59.976	18.489	1.00	17.91	A	C
ATOM	1490	CE2	TYR	211	57.306	60.065	17.716	1.00	18.80	A	C
ATOM	1491	CZ	TYR	211	58.221	61.063	17.979	1.00	18.36	A	C
ATOM	1492	OH	TYR	211	59.360	61.149	17.224	1.00	23.65	A	O
ATOM	1493	C	TYR	211	53.588	62.689	19.428	1.00	22.96	A	C
ATOM	1494	O	TYR	211	54.365	63.443	18.837	1.00	25.79	A	O
ATOM	1495	N	SER	212	52.365	62.433	18.983	1.00	20.96	A	N
ATOM	1496	CA	SER	212	51.918	63.033	17.746	1.00	19.56	A	C
ATOM	1497	CB	SER	212	50.835	62.175	17.090	1.00	20.97	A	C
ATOM	1498	OG	SER	212	49.635	62.208	17.829	1.00	21.79	A	O
ATOM	1499	C	SER	212	51.397	64.439	17.959	1.00	18.50	A	C
ATOM	1500	O	SER	212	50.933	64.789	19.040	1.00	16.31	A	O
ATOM	1501	N	ALA	213	51.493	65.236	16.901	1.00	17.84	A	N
ATOM	1502	CA	ALA	213	51.036	66.610	16.903	1.00	16.02	A	C
ATOM	1503	CB	ALA	213	52.193	67.548	17.224	1.00	14.16	A	C
ATOM	1504	C	ALA	213	50.429	66.935	15.526	1.00	15.57	A	C
ATOM	1505	O	ALA	213	50.857	67.862	14.833	1.00	13.25	A	O
ATOM	1506	N	LEU	214	49.448	66.132	15.129	1.00	14.75	A	N
ATOM	1507	CA	LEU	214	48.734	66.339	13.874	1.00	16.09	A	C
ATOM	1508	CB	LEU	214	49.353	65.517	12.735	1.00	16.40	A	C
ATOM	1509	CG	LEU	214	49.482	63.999	12.823	1.00	17.01	A	C
ATOM	1510	CD1	LEU	214	48.135	63.342	12.628	1.00	18.97	A	C
ATOM	1511	CD2	LEU	214	50.434	63.535	11.742	1.00	16.98	A	C
ATOM	1512	C	LEU	214	47.273	65.963	14.124	1.00	16.65	A	C
ATOM	1513	O	LEU	214	46.966	64.933	14.728	1.00	18.12	A	O
ATOM	1514	N	TRP	215	46.366	66.811	13.666	1.00	16.16	A	N
ATOM	1515	CA	TRP	215	44.959	66.590	13.907	1.00	14.69	A	C
ATOM	1516	CB	TRP	215	44.471	67.663	14.863	1.00	15.49	A	C
ATOM	1517	CG	TRP	215	45.230	67.669	16.145	1.00	17.52	A	C
ATOM	1518	CD2	TRP	215	46.482	68.325	16.403	1.00	17.74	A	C

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(Continued)

## FIG. 4 - 3 2

ATOM	1519	CE2	TRP	215	46.852	68.008	17.729	1.00	17.50	A	C
ATOM	1520	CE3	TRP	215	47.325	69.149	15.643	1.00	18.21	A	C
ATOM	1521	CD1	TRP	215	44.904	67.004	17.289	1.00	15.79	A	C
ATOM	1522	NE1	TRP	215	45.873	67.202	18.243	1.00	17.35	A	N
ATOM	1523	CZ2	TRP	215	48.033	68.485	18.318	1.00	18.06	A	C
ATOM	1524	CZ3	TRP	215	48.505	69.625	16.228	1.00	18.96	A	C
ATOM	1525	CH2	TRP	215	48.844	69.289	17.555	1.00	18.21	A	C
ATOM	1526	C	TRP	215	44.110	66.605	12.661	1.00	15.55	A	C
ATOM	1527	O	TRP	215	43.869	67.668	12.090	1.00	16.18	A	O
ATOM	1528	N	TRP	216	43.646	65.430	12.244	1.00	15.31	A	N
ATOM	1529	CA	TRP	216	42.793	65.330	11.069	1.00	16.40	A	C
ATOM	1530	CB	TRP	216	42.494	63.873	10.739	1.00	16.43	A	C
ATOM	1531	CG	TRP	216	43.549	63.114	10.002	1.00	17.38	A	C
ATOM	1532	CD2	TRP	216	43.823	63.169	8.599	1.00	17.01	A	C
ATOM	1533	CE2	TRP	216	44.794	62.176	8.320	1.00	17.25	A	C
ATOM	1534	CE3	TRP	216	43.340	63.954	7.549	1.00	17.09	A	C
ATOM	1535	CD1	TRP	216	44.352	62.125	10.508	1.00	18.55	A	C
ATOM	1536	NE1	TRP	216	45.098	61.553	9.501	1.00	18.07	A	N
ATOM	1537	CZ2	TRP	216	45.286	61.951	7.036	1.00	15.24	A	C
ATOM	1538	CZ3	TRP	216	43.829	63.729	6.270	1.00	17.06	A	C
ATOM	1539	CH2	TRP	216	44.794	62.734	6.027	1.00	17.07	A	C
ATOM	1540	C	TRP	216	41.461	66.016	11.355	1.00	17.17	A	C
ATOM	1541	O	TRP	216	40.990	66.005	12.487	1.00	18.00	A	O
ATOM	1542	N	SER	217	40.847	66.605	10.334	1.00	18.39	A	N
ATOM	1543	CA	SER	217	39.552	67.240	10.523	1.00	19.62	A	C
ATOM	1544	CB	SER	217	39.257	68.225	9.392	1.00	20.31	A	C
ATOM	1545	OG	SER	217	39.234	67.589	8.133	1.00	24.00	A	O
ATOM	1546	C	SER	217	38.528	66.108	10.550	1.00	20.47	A	C
ATOM	1547	O	SER	217	38.814	64.994	10.110	1.00	20.32	A	O
ATOM	1548	N	PRO	218	37.326	66.369	11.074	1.00	20.82	A	N
ATOM	1549	CD	PRO	218	36.827	67.650	11.598	1.00	20.28	A	C
ATOM	1550	CA	PRO	218	36.285	65.339	11.154	1.00	22.67	A	C
ATOM	1551	CB	PRO	218	35.033	66.148	11.462	1.00	21.68	A	C
ATOM	1552	CG	PRO	218	35.587	67.223	12.353	1.00	21.12	A	C
ATOM	1553	C	PRO	218	36.123	64.404	9.950	1.00	23.46	A	C
ATOM	1554	O	PRO	218	36.190	63.183	10.107	1.00	25.13	A	O
ATOM	1555	N	ASN	219	35.909	64.948	8.756	1.00	22.93	A	N
ATOM	1556	CA	ASN	219	35.756	64.071	7.600	1.00	22.31	A	C
ATOM	1557	CB	ASN	219	34.704	64.622	6.631	1.00	22.48	A	C
ATOM	1558	CG	ASN	219	35.172	65.849	5.903	1.00	24.12	A	C
ATOM	1559	OD1	ASN	219	36.373	66.076	5.760	1.00	26.01	A	O
ATOM	1560	ND2	ASN	219	34.230	66.640	5.411	1.00	26.27	A	N
ATOM	1561	C	ASN	219	37.090	63.841	6.871	1.00	21.20	A	C
ATOM	1562	O	ASN	219	37.115	63.307	5.760	1.00	20.94	A	O
ATOM	1563	N	GLY	220	38.184	64.267	7.499	1.00	18.33	A	N
ATOM	1564	CA	GLY	220	39.512	64.068	6.941	1.00	17.97	A	C
ATOM	1565	C	GLY	220	40.035	64.993	5.853	1.00	18.92	A	C
ATOM	1566	O	GLY	220	41.157	64.801	5.375	1.00	20.28	A	O
ATOM	1567	N	THR	221	39.242	65.980	5.447	1.00	17.57	A	N

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(Continued)

## FIG. 4 - 33

ATOM	1568	CA	THR	221	39.654	66.917	4.408	1.00	15.80	A	C
ATOM	1569	CB	THR	221	38.540	67.942	4.112	1.00	15.67	A	C
ATOM	1570	OG1	THR	221	37.410	67.269	3.550	1.00	16.41	A	O
ATOM	1571	CG2	THR	221	39.019	69.004	3.147	1.00	12.96	A	C
ATOM	1572	C	THR	221	40.903	67.674	4.833	1.00	16.70	A	C
ATOM	1573	O	THR	221	41.884	67.753	4.088	1.00	16.98	A	O
ATOM	1574	N	PHE	222	40.864	68.238	6.033	1.00	15.92	A	N
ATOM	1575	CA	PHE	222	41.999	69.001	6.539	1.00	15.88	A	C
ATOM	1576	CB	PHE	222	41.508	70.253	7.262	1.00	15.20	A	C
ATOM	1577	CG	PHE	222	40.939	71.305	6.356	1.00	14.35	A	C
ATOM	1578	CD1	PHE	222	39.569	71.542	6.323	1.00	11.89	A	C
ATOM	1579	CD2	PHE	222	41.782	72.097	5.571	1.00	14.45	A	C
ATOM	1580	CE1	PHE	222	39.046	72.550	5.533	1.00	13.50	A	C
ATOM	1581	CE2	PHE	222	41.269	73.112	4.771	1.00	12.61	A	C
ATOM	1582	CZ	PHE	222	39.897	73.342	4.751	1.00	15.23	A	C
ATOM	1583	C	PHE	222	42.907	68.228	7.494	1.00	16.13	A	C
ATOM	1584	O	PHE	222	42.467	67.327	8.211	1.00	16.82	A	O
ATOM	1585	N	LEU	223	44.187	68.582	7.484	1.00	15.93	A	N
ATOM	1586	CA	LEU	223	45.159	67.983	8.385	1.00	14.81	A	C
ATOM	1587	CB	LEU	223	46.199	67.142	7.645	1.00	14.64	A	C
ATOM	1588	CG	LEU	223	47.306	66.627	8.584	1.00	14.94	A	C
ATOM	1589	CD1	LEU	223	46.696	65.773	9.687	1.00	11.99	A	C
ATOM	1590	CD2	LEU	223	48.338	65.830	7.808	1.00	11.50	A	C
ATOM	1591	C	LEU	223	45.848	69.162	9.031	1.00	16.80	A	C
ATOM	1592	O	LEU	223	46.398	70.028	8.341	1.00	16.53	A	O
ATOM	1593	N	ALA	224	45.790	69.219	10.353	1.00	17.34	A	N
ATOM	1594	CA	ALA	224	46.420	70.308	11.073	1.00	18.47	A	C
ATOM	1595	CB	ALA	224	45.422	70.950	12.029	1.00	17.47	A	C
ATOM	1596	C	ALA	224	47.596	69.735	11.840	1.00	18.77	A	C
ATOM	1597	O	ALA	224	47.587	68.561	12.205	1.00	19.22	A	O
ATOM	1598	N	TYR	225	48.614	70.551	12.078	1.00	17.68	A	N
ATOM	1599	CA	TYR	225	49.764	70.068	12.819	1.00	17.56	A	C
ATOM	1600	CB	TYR	225	50.726	69.306	11.891	1.00	16.48	A	C
ATOM	1601	CG	TYR	225	51.273	70.108	10.726	1.00	15.05	A	C
ATOM	1602	CD1	TYR	225	50.551	70.235	9.533	1.00	13.44	A	C
ATOM	1603	CE1	TYR	225	51.050	70.968	8.456	1.00	9.19	A	C
ATOM	1604	CD2	TYR	225	52.514	70.740	10.814	1.00	14.42	A	C
ATOM	1605	CE2	TYR	225	53.025	71.476	9.744	1.00	14.09	A	C
ATOM	1606	CZ	TYR	225	52.286	71.583	8.567	1.00	14.11	A	C
ATOM	1607	OH	TYR	225	52.802	72.292	7.504	1.00	14.49	A	O
ATOM	1608	C	TYR	225	50.514	71.182	13.521	1.00	17.79	A	C
ATOM	1609	O	TYR	225	50.326	72.359	13.229	1.00	19.91	A	O
ATOM	1610	N	ALA	226	51.358	70.796	14.462	1.00	17.65	A	N
ATOM	1611	CA	ALA	226	52.164	71.748	15.201	1.00	17.74	A	C
ATOM	1612	CB	ALA	226	52.060	71.472	16.687	1.00	18.89	A	C
ATOM	1613	C	ALA	226	53.601	71.575	14.740	1.00	17.39	A	C
ATOM	1614	O	ALA	226	53.966	70.527	14.204	1.00	16.05	A	O
ATOM	1615	N	GLN	227	54.412	72.606	14.941	1.00	17.45	A	N
ATOM	1616	CA	GLN	227	55.816	72.552	14.555	1.00	16.64	A	C

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(Continued)

## FIG. 4 - 34

ATOM	1617	CB	GLN	227	56.096	73.423	13.331	1.00	15.62	A	C
ATOM	1618	CG	GLN	227	57.514	73.246	12.799	1.00	16.35	A	C
ATOM	1619	CD	GLN	227	57.847	74.191	11.666	1.00	14.31	A	C
ATOM	1620	OE1	GLN	227	57.877	75.408	11.851	1.00	18.11	A	O
ATOM	1621	NE2	GLN	227	58.101	73.639	10.486	1.00	12.45	A	N
ATOM	1622	C	GLN	227	56.615	73.073	15.723	1.00	16.27	A	C
ATOM	1623	O	GLN	227	56.346	74.159	16.225	1.00	16.33	A	O
ATOM	1624	N	PHE	228	57.601	72.301	16.158	1.00	17.36	A	N
ATOM	1625	CA	PHE	228	58.414	72.717	17.287	1.00	16.81	A	C
ATOM	1626	CB	PHE	228	58.327	71.686	18.412	1.00	14.62	A	C
ATOM	1627	CG	PHE	228	56.919	71.295	18.758	1.00	14.48	A	C
ATOM	1628	CD1	PHE	228	56.317	70.196	18.141	1.00	14.37	A	C
ATOM	1629	CD2	PHE	228	56.183	72.036	19.674	1.00	12.73	A	C
ATOM	1630	CE1	PHE	228	55.007	69.840	18.430	1.00	13.56	A	C
ATOM	1631	CE2	PHE	228	54.870	71.691	19.971	1.00	14.73	A	C
ATOM	1632	CZ	PHE	228	54.279	70.588	19.348	1.00	15.31	A	C
ATOM	1633	C	PHE	228	59.848	72.922	16.859	1.00	18.12	A	C
ATOM	1634	O	PHE	228	60.410	72.121	16.112	1.00	17.47	A	O
ATOM	1635	N	ASN	229	60.413	74.027	17.335	1.00	20.00	A	N
ATOM	1636	CA	ASN	229	61.779	74.435	17.042	1.00	20.87	A	C
ATOM	1637	CB	ASN	229	61.767	75.857	16.474	1.00	21.57	A	C
ATOM	1638	CG	ASN	229	63.086	76.257	15.870	1.00	24.35	A	C
ATOM	1639	OD1	ASN	229	64.141	75.774	16.289	1.00	26.00	A	O
ATOM	1640	ND2	ASN	229	63.025	77.153	14.887	1.00	25.62	A	N
ATOM	1641	C	ASN	229	62.540	74.421	18.362	1.00	21.39	A	C
ATOM	1642	O	ASN	229	62.232	75.200	19.269	1.00	21.52	A	O
ATOM	1643	N	ASP	230	63.516	73.530	18.481	1.00	20.96	A	N
ATOM	1644	CA	ASP	230	64.300	73.444	19.706	1.00	22.78	A	C
ATOM	1645	CB	ASP	230	64.275	72.026	20.268	1.00	22.69	A	C
ATOM	1646	CG	ASP	230	62.880	71.551	20.580	1.00	22.37	A	C
ATOM	1647	OD1	ASP	230	62.681	71.015	21.689	1.00	21.57	A	O
ATOM	1648	OD2	ASP	230	61.993	71.705	19.713	1.00	21.82	A	O
ATOM	1649	C	ASP	230	65.734	73.825	19.412	1.00	24.50	A	C
ATOM	1650	O	ASP	230	66.663	73.252	19.979	1.00	24.72	A	O
ATOM	1651	N	THR	231	65.904	74.803	18.527	1.00	25.87	A	N
ATOM	1652	CA	THR	231	67.228	75.245	18.122	1.00	26.22	A	C
ATOM	1653	CB	THR	231	67.149	76.406	17.109	1.00	27.87	A	C
ATOM	1654	OG1	THR	231	66.540	75.947	15.893	1.00	28.62	A	O
ATOM	1655	CG2	THR	231	68.545	76.947	16.813	1.00	26.63	A	C
ATOM	1656	C	THR	231	68.099	75.688	19.280	1.00	26.77	A	C
ATOM	1657	O	THR	231	69.254	75.277	19.375	1.00	27.34	A	O
ATOM	1658	N	GLU	232	67.550	76.519	20.163	1.00	25.50	A	N
ATOM	1659	CA	GLU	232	68.329	77.020	21.285	1.00	24.52	A	C
ATOM	1660	CB	GLU	232	68.154	78.526	21.397	1.00	28.36	A	C
ATOM	1661	CG	GLU	232	68.615	79.281	20.171	1.00	34.72	A	C
ATOM	1662	CD	GLU	232	68.483	80.780	20.338	1.00	40.02	A	C
ATOM	1663	OE1	GLU	232	68.767	81.509	19.363	1.00	44.21	A	O
ATOM	1664	OE2	GLU	232	68.100	81.232	21.444	1.00	42.26	A	O
ATOM	1665	C	GLU	232	68.020	76.377	22.627	1.00	22.97	A	C

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(Continued)

## FIG. 4 - 35

ATOM	1666	O	GLU	232	68.331	76.942	23.679	1.00	20.81	A	O
ATOM	1667	N	VAL	233	67.416	75.194	22.596	1.00	20.32	A	N
ATOM	1668	CA	VAL	233	67.091	74.499	23.832	1.00	17.88	A	C
ATOM	1669	CB	VAL	233	65.853	73.618	23.648	1.00	17.88	A	C
ATOM	1670	CG1	VAL	233	65.522	72.925	24.957	1.00	14.00	A	C
ATOM	1671	CG2	VAL	233	64.678	74.478	23.160	1.00	16.73	A	C
ATOM	1672	C	VAL	233	68.261	73.642	24.304	1.00	16.00	A	C
ATOM	1673	O	VAL	233	68.694	72.728	23.606	1.00	15.94	A	O
ATOM	1674	N	PRO	234	68.788	73.927	25.504	1.00	14.51	A	N
ATOM	1675	CD	PRO	234	68.313	74.907	26.494	1.00	13.03	A	C
ATOM	1676	CA	PRO	234	69.914	73.162	26.040	1.00	13.93	A	C
ATOM	1677	CB	PRO	234	70.031	73.677	27.473	1.00	12.63	A	C
ATOM	1678	CG	PRO	234	69.517	75.059	27.377	1.00	11.32	A	C
ATOM	1679	C	PRO	234	69.643	71.663	25.987	1.00	16.20	A	C
ATOM	1680	O	PRO	234	68.487	71.220	26.041	1.00	15.73	A	O
ATOM	1681	N	LEU	235	70.716	70.887	25.900	1.00	16.28	A	N
ATOM	1682	CA	LEU	235	70.602	69.443	25.825	1.00	16.91	A	C
ATOM	1683	CB	LEU	235	71.505	68.912	24.718	1.00	18.54	A	C
ATOM	1684	CG	LEU	235	71.267	69.349	23.273	1.00	21.93	A	C
ATOM	1685	CD1	LEU	235	72.434	68.856	22.412	1.00	21.90	A	C
ATOM	1686	CD2	LEU	235	69.946	68.790	22.768	1.00	19.17	A	C
ATOM	1687	C	LEU	235	70.990	68.743	27.118	1.00	17.26	A	C
ATOM	1688	O	LEU	235	71.939	69.157	27.793	1.00	18.36	A	O
ATOM	1689	N	ILE	236	70.244	67.696	27.472	1.00	14.95	A	N
ATOM	1690	CA	ILE	236	70.586	66.899	28.644	1.00	12.68	A	C
ATOM	1691	CB	ILE	236	69.345	66.245	29.335	1.00	10.50	A	C
ATOM	1692	CG2	ILE	236	68.538	65.433	28.329	1.00	9.32	A	C
ATOM	1693	CG1	ILE	236	69.806	65.298	30.448	1.00	8.74	A	C
ATOM	1694	CD1	ILE	236	70.789	65.919	31.427	1.00	7.11	A	C
ATOM	1695	C	ILE	236	71.444	65.802	28.010	1.00	12.84	A	C
ATOM	1696	O	ILE	236	71.105	65.276	26.942	1.00	10.11	A	O
ATOM	1697	N	GLU	237	72.558	65.480	28.650	1.00	12.44	A	N
ATOM	1698	CA	GLU	237	73.463	64.470	28.128	1.00	14.46	A	C
ATOM	1699	CB	GLU	237	74.767	65.128	27.655	1.00	13.45	A	C
ATOM	1700	CG	GLU	237	74.554	66.079	26.500	1.00	18.02	A	C
ATOM	1701	CD	GLU	237	75.845	66.500	25.819	1.00	23.46	A	C
ATOM	1702	OE1	GLU	237	75.779	67.016	24.683	1.00	25.80	A	O
ATOM	1703	OE2	GLU	237	76.928	66.324	26.408	1.00	26.23	A	O
ATOM	1704	C	GLU	237	73.744	63.427	29.191	1.00	13.41	A	C
ATOM	1705	O	GLU	237	73.895	63.752	30.363	1.00	14.43	A	O
ATOM	1706	N	TYR	238	73.801	62.169	28.781	1.00	12.83	A	N
ATOM	1707	CA	TYR	238	74.052	61.093	29.721	1.00	14.06	A	C
ATOM	1708	CB	TYR	238	72.810	60.840	30.595	1.00	12.42	A	C
ATOM	1709	CG	TYR	238	71.566	60.419	29.856	1.00	11.79	A	C
ATOM	1710	CD1	TYR	238	71.451	59.139	29.317	1.00	16.12	A	C
ATOM	1711	CE1	TYR	238	70.292	58.739	28.635	1.00	17.09	A	C
ATOM	1712	CD2	TYR	238	70.496	61.295	29.701	1.00	12.13	A	C
ATOM	1713	CE2	TYR	238	69.336	60.913	29.020	1.00	12.94	A	C
ATOM	1714	CZ	TYR	238	69.243	59.634	28.487	1.00	15.48	A	C

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(Continued)

## FIG. 4 - 36

ATOM	1715	OH	TYR	238	68.127	59.257	27.775	1.00	15.96	A	O
ATOM	1716	C	TYR	238	74.445	59.847	28.954	1.00	15.25	A	C
ATOM	1717	O	TYR	238	74.059	59.667	27.798	1.00	17.74	A	O
ATOM	1718	N	SER	239	75.220	58.986	29.596	1.00	14.10	A	N
ATOM	1719	CA	SER	239	75.689	57.779	28.943	1.00	13.87	A	C
ATOM	1720	CB	SER	239	76.926	57.251	29.656	1.00	11.90	A	C
ATOM	1721	OG	SER	239	77.902	58.265	29.766	1.00	18.76	A	O
ATOM	1722	C	SER	239	74.661	56.668	28.879	1.00	13.45	A	C
ATOM	1723	O	SER	239	73.755	56.587	29.700	1.00	14.39	A	O
ATOM	1724	N	PHE	240	74.809	55.834	27.862	1.00	12.12	A	N
ATOM	1725	CA	PHE	240	73.972	54.678	27.679	1.00	12.95	A	C
ATOM	1726	CB	PHE	240	73.003	54.833	26.523	1.00	12.48	A	C
ATOM	1727	CG	PHE	240	71.896	53.843	26.574	1.00	11.50	A	C
ATOM	1728	CD1	PHE	240	70.824	54.037	27.436	1.00	10.15	A	C
ATOM	1729	CD2	PHE	240	71.980	52.655	25.858	1.00	11.95	A	C
ATOM	1730	CE1	PHE	240	69.859	53.064	27.597	1.00	10.78	A	C
ATOM	1731	CE2	PHE	240	71.018	51.675	26.012	1.00	11.03	A	C
ATOM	1732	CZ	PHE	240	69.954	51.878	26.888	1.00	10.46	A	C
ATOM	1733	C	PHE	240	75.018	53.652	27.330	1.00	14.83	A	C
ATOM	1734	O	PHE	240	75.722	53.805	26.335	1.00	18.18	A	O
ATOM	1735	N	TYR	241	75.129	52.617	28.153	1.00	13.74	A	N
ATOM	1736	CA	TYR	241	76.147	51.612	27.958	1.00	13.29	A	C
ATOM	1737	CB	TYR	241	76.526	51.057	29.329	1.00	13.69	A	C
ATOM	1738	CG	TYR	241	76.833	52.167	30.317	1.00	10.88	A	C
ATOM	1739	CD1	TYR	241	78.065	52.821	30.308	1.00	11.93	A	C
ATOM	1740	CE1	TYR	241	78.326	53.894	31.168	1.00	9.47	A	C
ATOM	1741	CD2	TYR	241	75.862	52.610	31.218	1.00	12.15	A	C
ATOM	1742	CE2	TYR	241	76.106	53.678	32.080	1.00	11.02	A	C
ATOM	1743	CZ	TYR	241	77.338	54.319	32.046	1.00	12.15	A	C
ATOM	1744	OH	TYR	241	77.556	55.408	32.859	1.00	10.38	A	O
ATOM	1745	C	TYR	241	75.793	50.510	26.967	1.00	14.62	A	C
ATOM	1746	O	TYR	241	76.686	49.948	26.322	1.00	12.20	A	O
ATOM	1747	N	SER	242	74.501	50.204	26.837	1.00	16.13	A	N
ATOM	1748	CA	SER	242	74.053	49.180	25.888	1.00	16.13	A	C
ATOM	1749	CB	SER	242	74.464	49.590	24.469	1.00	16.30	A	C
ATOM	1750	OG	SER	242	74.004	48.674	23.496	1.00	17.85	A	O
ATOM	1751	C	SER	242	74.647	47.816	26.226	1.00	17.46	A	C
ATOM	1752	O	SER	242	75.219	47.625	27.303	1.00	19.13	A	O
ATOM	1753	N	ASP	243	74.516	46.865	25.312	1.00	19.34	A	N
ATOM	1754	CA	ASP	243	75.066	45.535	25.548	1.00	23.36	A	C
ATOM	1755	CB	ASP	243	74.774	44.605	24.369	1.00	27.30	A	C
ATOM	1756	CG	ASP	243	73.290	44.419	24.132	1.00	33.83	A	C
ATOM	1757	OD1	ASP	243	72.549	44.246	25.126	1.00	36.97	A	O
ATOM	1758	OD2	ASP	243	72.862	44.438	22.955	1.00	37.15	A	O
ATOM	1759	C	ASP	243	76.572	45.554	25.805	1.00	23.56	A	C
ATOM	1760	O	ASP	243	77.298	46.432	25.330	1.00	22.48	A	O
ATOM	1761	N	GLU	244	77.016	44.559	26.567	1.00	24.45	A	N
ATOM	1762	CA	GLU	244	78.412	44.363	26.944	1.00	22.80	A	C
ATOM	1763	CB	GLU	244	78.534	42.984	27.605	1.00	23.73	A	C

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(Continued)

## FIG. 4 - 37

ATOM	1764	CG	GLU	244	79.940	42.547	27.995	1.00	29.35	A	C
ATOM	1765	CD	GLU	244	79.967	41.177	28.667	1.00	29.80	A	C
ATOM	1766	OE1	GLU	244	81.079	40.680	28.958	1.00	29.53	A	O
ATOM	1767	OE2	GLU	244	78.877	40.601	28.903	1.00	29.32	A	O
ATOM	1768	C	GLU	244	79.374	44.476	25.754	1.00	22.28	A	C
ATOM	1769	O	GLU	244	80.533	44.854	25.913	1.00	21.94	A	O
ATOM	1770	N	SER	245	78.888	44.159	24.561	1.00	21.62	A	N
ATOM	1771	CA	SER	245	79.724	44.205	23.370	1.00	19.92	A	C
ATOM	1772	CB	SER	245	79.080	43.402	22.244	1.00	19.31	A	C
ATOM	1773	OG	SER	245	77.949	44.068	21.723	1.00	17.93	A	O
ATOM	1774	C	SER	245	80.044	45.605	22.861	1.00	19.58	A	C
ATOM	1775	O	SER	245	80.874	45.762	21.971	1.00	21.35	A	O
ATOM	1776	N	LEU	246	79.392	46.628	23.397	1.00	18.69	A	N
ATOM	1777	CA	LEU	246	79.694	47.983	22.943	1.00	18.41	A	C
ATOM	1778	CB	LEU	246	78.522	48.926	23.229	1.00	18.20	A	C
ATOM	1779	CG	LEU	246	78.659	50.368	22.728	1.00	17.99	A	C
ATOM	1780	CD1	LEU	246	78.736	50.388	21.214	1.00	16.83	A	C
ATOM	1781	CD2	LEU	246	77.458	51.181	23.192	1.00	19.98	A	C
ATOM	1782	C	LEU	246	80.943	48.463	23.679	1.00	18.12	A	C
ATOM	1783	O	LEU	246	80.921	48.662	24.895	1.00	16.81	A	O
ATOM	1784	N	GLN	247	82.034	48.635	22.940	1.00	17.84	A	N
ATOM	1785	CA	GLN	247	83.295	49.073	23.532	1.00	17.30	A	C
ATOM	1786	CB	GLN	247	84.400	49.038	22.480	1.00	15.11	A	C
ATOM	1787	CG	GLN	247	85.791	49.234	23.045	1.00	17.62	A	C
ATOM	1788	CD	GLN	247	86.875	48.770	22.090	1.00	18.47	A	C
ATOM	1789	OE1	GLN	247	86.829	49.065	20.899	1.00	20.53	A	O
ATOM	1790	NE2	GLN	247	87.862	48.049	22.611	1.00	17.76	A	N
ATOM	1791	C	GLN	247	83.224	50.461	24.170	1.00	17.66	A	C
ATOM	1792	O	GLN	247	83.640	50.648	25.313	1.00	17.56	A	O
ATOM	1793	N	TYR	248	82.710	51.436	23.430	1.00	18.50	A	N
ATOM	1794	CA	TYR	248	82.592	52.794	23.954	1.00	19.00	A	C
ATOM	1795	CB	TYR	248	83.177	53.822	22.972	1.00	17.39	A	C
ATOM	1796	CG	TYR	248	84.684	53.820	22.860	1.00	16.80	A	C
ATOM	1797	CD1	TYR	248	85.353	52.812	22.172	1.00	17.20	A	C
ATOM	1798	CE1	TYR	248	86.742	52.814	22.058	1.00	17.58	A	C
ATOM	1799	CD2	TYR	248	85.444	54.838	23.437	1.00	17.77	A	C
ATOM	1800	CE2	TYR	248	86.839	54.851	23.333	1.00	17.22	A	C
ATOM	1801	CZ	TYR	248	87.479	53.836	22.647	1.00	18.42	A	C
ATOM	1802	OH	TYR	248	88.854	53.809	22.595	1.00	19.27	A	O
ATOM	1803	C	TYR	248	81.130	53.134	24.212	1.00	18.87	A	C
ATOM	1804	O	TYR	248	80.288	53.018	23.323	1.00	19.15	A	O
ATOM	1805	N	PRO	249	80.804	53.549	25.440	1.00	18.20	A	N
ATOM	1806	CD	PRO	249	81.610	53.595	26.668	1.00	18.21	A	C
ATOM	1807	CA	PRO	249	79.411	53.886	25.716	1.00	18.83	A	C
ATOM	1808	CB	PRO	249	79.424	54.222	27.206	1.00	19.46	A	C
ATOM	1809	CG	PRO	249	80.857	54.582	27.481	1.00	17.63	A	C
ATOM	1810	C	PRO	249	78.937	55.042	24.852	1.00	19.66	A	C
ATOM	1811	O	PRO	249	79.734	55.864	24.413	1.00	20.92	A	O
ATOM	1812	N	LYS	250	77.638	55.096	24.599	1.00	19.01	A	N

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(Continued)

## FIG. 4 - 38

ATOM	1813	CA	LYS	250	77.083	56.158	23.785	1.00	19.61	A	C
ATOM	1814	CB	LYS	250	75.933	55.618	22.936	1.00	23.51	A	C
ATOM	1815	CG	LYS	250	76.320	54.428	22.089	1.00	28.40	A	C
ATOM	1816	CD	LYS	250	75.197	54.010	21.152	1.00	30.62	A	C
ATOM	1817	CE	LYS	250	75.698	52.938	20.203	1.00	32.02	A	C
ATOM	1818	NZ	LYS	250	76.966	53.385	19.546	1.00	32.62	A	N
ATOM	1819	C	LYS	250	76.580	57.320	24.628	1.00	17.92	A	C
ATOM	1820	O	LYS	250	76.130	57.130	25.758	1.00	17.90	A	O
ATOM	1821	N	THR	251	76.663	58.524	24.077	1.00	14.61	A	N
ATOM	1822	CA	THR	251	76.171	59.689	24.786	1.00	15.48	A	C
ATOM	1823	CB	THR	251	77.104	60.887	24.666	1.00	13.61	A	C
ATOM	1824	OG1	THR	251	78.280	60.654	25.441	1.00	15.96	A	O
ATOM	1825	CG2	THR	251	76.414	62.137	25.181	1.00	13.93	A	C
ATOM	1826	C	THR	251	74.832	60.086	24.205	1.00	16.04	A	C
ATOM	1827	O	THR	251	74.755	60.572	23.083	1.00	17.34	A	O
ATOM	1828	N	VAL	252	73.779	59.860	24.977	1.00	15.27	A	N
ATOM	1829	CA	VAL	252	72.439	60.205	24.559	1.00	16.08	A	C
ATOM	1830	CB	VAL	252	71.405	59.381	25.355	1.00	16.76	A	C
ATOM	1831	CG1	VAL	252	69.987	59.832	25.014	1.00	16.29	A	C
ATOM	1832	CG2	VAL	252	71.595	57.895	25.050	1.00	13.65	A	C
ATOM	1833	C	VAL	252	72.223	61.699	24.799	1.00	18.46	A	C
ATOM	1834	O	VAL	252	72.443	62.212	25.905	1.00	19.01	A	O
ATOM	1835	N	ARG	253	71.799	62.398	23.754	1.00	19.18	A	N
ATOM	1836	CA	ARG	253	71.568	63.831	23.842	1.00	18.54	A	C
ATOM	1837	CB	ARG	253	72.574	64.567	22.949	1.00	19.46	A	C
ATOM	1838	CG	ARG	253	74.014	64.439	23.457	1.00	24.49	A	C
ATOM	1839	CD	ARG	253	75.021	65.066	22.519	1.00	29.04	A	C
ATOM	1840	NE	ARG	253	75.797	64.044	21.822	1.00	35.89	A	N
ATOM	1841	CZ	ARG	253	77.013	63.647	22.185	1.00	38.08	A	C
ATOM	1842	NH1	ARG	253	77.606	64.191	23.241	1.00	39.69	A	N
ATOM	1843	NH2	ARG	253	77.633	62.699	21.497	1.00	40.12	A	N
ATOM	1844	C	ARG	253	70.140	64.156	23.449	1.00	17.33	A	C
ATOM	1845	O	ARG	253	69.690	63.802	22.362	1.00	18.44	A	O
ATOM	1846	N	VAL	254	69.432	64.836	24.344	1.00	16.85	A	N
ATOM	1847	CA	VAL	254	68.033	65.196	24.125	1.00	15.67	A	C
ATOM	1848	CB	VAL	254	67.079	64.405	25.070	1.00	16.67	A	C
ATOM	1849	CG1	VAL	254	65.640	64.775	24.766	1.00	16.79	A	C
ATOM	1850	CG2	VAL	254	67.308	62.899	24.951	1.00	17.24	A	C
ATOM	1851	C	VAL	254	67.737	66.660	24.405	1.00	14.62	A	C
ATOM	1852	O	VAL	254	68.122	67.186	25.450	1.00	15.12	A	O
ATOM	1853	N	PRO	255	67.048	67.340	23.475	1.00	13.71	A	N
ATOM	1854	CD	PRO	255	66.677	66.945	22.105	1.00	10.62	A	C
ATOM	1855	CA	PRO	255	66.725	68.749	23.730	1.00	13.00	A	C
ATOM	1856	CB	PRO	255	66.064	69.193	22.431	1.00	13.28	A	C
ATOM	1857	CG	PRO	255	66.674	68.265	21.397	1.00	13.45	A	C
ATOM	1858	C	PRO	255	65.735	68.674	24.899	1.00	13.86	A	C
ATOM	1859	O	PRO	255	64.663	68.086	24.772	1.00	13.58	A	O
ATOM	1860	N	TYR	256	66.108	69.255	26.032	1.00	13.63	A	N
ATOM	1861	CA	TYR	256	65.304	69.194	27.242	1.00	11.65	A	C

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(Continued)

## FIG. 4 - 39

ATOM	1862	CB	TYR	256	65.801	68.006	28.077	1.00	10.57	A	C
ATOM	1863	CG	TYR	256	65.044	67.706	29.351	1.00	10.49	A	C
ATOM	1864	CD1	TYR	256	64.949	68.646	30.378	1.00	9.61	A	C
ATOM	1865	CE1	TYR	256	64.296	68.351	31.571	1.00	7.54	A	C
ATOM	1866	CD2	TYR	256	64.460	66.460	29.549	1.00	9.65	A	C
ATOM	1867	CE2	TYR	256	63.799	66.156	30.735	1.00	11.05	A	C
ATOM	1868	CZ	TYR	256	63.722	67.105	31.742	1.00	10.10	A	C
ATOM	1869	OH	TYR	256	63.060	66.801	32.909	1.00	10.49	A	O
ATOM	1870	C	TYR	256	65.488	70.492	28.012	1.00	12.70	A	C
ATOM	1871	O	TYR	256	66.559	70.750	28.553	1.00	15.49	A	O
ATOM	1872	N	PRO	257	64.444	71.325	28.080	1.00	12.39	A	N
ATOM	1873	CD	PRO	257	63.174	71.254	27.334	1.00	13.82	A	C
ATOM	1874	CA	PRO	257	64.548	72.593	28.800	1.00	11.47	A	C
ATOM	1875	CB	PRO	257	63.501	73.450	28.106	1.00	12.01	A	C
ATOM	1876	CG	PRO	257	62.405	72.464	27.866	1.00	12.87	A	C
ATOM	1877	C	PRO	257	64.296	72.489	30.298	1.00	12.85	A	C
ATOM	1878	O	PRO	257	63.174	72.210	30.723	1.00	15.59	A	O
ATOM	1879	N	LYS	258	65.327	72.718	31.105	1.00	11.64	A	N
ATOM	1880	CA	LYS	258	65.155	72.671	32.546	1.00	11.10	A	C
ATOM	1881	CB	LYS	258	66.501	72.439	33.227	1.00	12.96	A	C
ATOM	1882	CG	LYS	258	67.034	71.012	33.031	1.00	14.20	A	C
ATOM	1883	CD	LYS	258	68.519	70.906	33.331	1.00	13.34	A	C
ATOM	1884	CE	LYS	258	69.042	69.480	33.136	1.00	13.95	A	C
ATOM	1885	NZ	LYS	258	68.671	68.536	34.223	1.00	10.80	A	N
ATOM	1886	C	LYS	258	64.517	73.984	33.011	1.00	12.44	A	C
ATOM	1887	O	LYS	258	64.368	74.921	32.224	1.00	11.13	A	O
ATOM	1888	N	ALA	259	64.124	74.043	34.280	1.00	13.33	A	N
ATOM	1889	CA	ALA	259	63.484	75.236	34.844	1.00	14.81	A	C
ATOM	1890	CB	ALA	259	63.368	75.097	36.355	1.00	16.40	A	C
ATOM	1891	C	ALA	259	64.167	76.555	34.508	1.00	15.14	A	C
ATOM	1892	O	ALA	259	65.317	76.787	34.881	1.00	17.32	A	O
ATOM	1893	N	GLY	260	63.448	77.419	33.802	1.00	16.82	A	N
ATOM	1894	CA	GLY	260	63.984	78.720	33.444	1.00	15.59	A	C
ATOM	1895	C	GLY	260	64.870	78.749	32.217	1.00	15.78	A	C
ATOM	1896	O	GLY	260	65.379	79.812	31.852	1.00	17.65	A	O
ATOM	1897	N	ALA	261	65.072	77.600	31.577	1.00	13.77	A	N
ATOM	1898	CA	ALA	261	65.906	77.554	30.379	1.00	11.19	A	C
ATOM	1899	CB	ALA	261	66.524	76.182	30.224	1.00	10.21	A	C
ATOM	1900	C	ALA	261	65.093	77.911	29.137	1.00	10.04	A	C
ATOM	1901	O	ALA	261	63.896	78.160	29.212	1.00	8.71	A	O
ATOM	1902	N	VAL	262	65.747	77.947	27.987	1.00	11.73	A	N
ATOM	1903	CA	VAL	262	65.050	78.284	26.761	1.00	12.13	A	C
ATOM	1904	CB	VAL	262	66.035	78.529	25.594	1.00	11.50	A	C
ATOM	1905	CG1	VAL	262	65.257	78.796	24.299	1.00	8.31	A	C
ATOM	1906	CG2	VAL	262	66.939	79.732	25.920	1.00	5.79	A	C
ATOM	1907	C	VAL	262	64.092	77.167	26.389	1.00	13.92	A	C
ATOM	1908	O	VAL	262	64.471	76.001	26.341	1.00	16.73	A	O
ATOM	1909	N	ASN	263	62.844	77.536	26.139	1.00	13.49	A	N
ATOM	1910	CA	ASN	263	61.816	76.585	25.773	1.00	13.67	A	C

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ATOM	1911	CB	ASN	263	60.470	77.038	26.336	1.00	14.53	A	C
ATOM	1912	CG	ASN	263	60.222	76.545	27.746	1.00	17.27	A	C
ATOM	1913	OD1	ASN	263	59.342	77.058	28.444	1.00	18.62	A	O
ATOM	1914	ND2	ASN	263	60.977	75.534	28.169	1.00	16.78	A	N
ATOM	1915	C	ASN	263	61.715	76.500	24.265	1.00	14.45	A	C
ATOM	1916	O	ASN	263	62.170	77.395	23.561	1.00	16.33	A	O
ATOM	1917	N	PRO	264	61.119	75.418	23.743	1.00	14.86	A	N
ATOM	1918	CD	PRO	264	60.513	74.254	24.412	1.00	15.86	A	C
ATOM	1919	CA	PRO	264	60.986	75.301	22.294	1.00	15.41	A	C
ATOM	1920	CB	PRO	264	60.591	73.844	22.106	1.00	14.97	A	C
ATOM	1921	CG	PRO	264	59.721	73.607	23.287	1.00	14.81	A	C
ATOM	1922	C	PRO	264	59.867	76.238	21.882	1.00	15.66	A	C
ATOM	1923	O	PRO	264	58.954	76.496	22.663	1.00	17.42	A	O
ATOM	1924	N	THR	265	59.942	76.767	20.673	1.00	15.76	A	N
ATOM	1925	CA	THR	265	58.895	77.648	20.199	1.00	14.67	A	C
ATOM	1926	CB	THR	265	59.458	78.779	19.341	1.00	15.37	A	C
ATOM	1927	OG1	THR	265	60.162	78.228	18.223	1.00	15.98	A	O
ATOM	1928	CG2	THR	265	60.402	79.633	20.159	1.00	12.01	A	C
ATOM	1929	C	THR	265	58.024	76.749	19.360	1.00	15.62	A	C
ATOM	1930	O	THR	265	58.465	75.683	18.932	1.00	18.75	A	O
ATOM	1931	N	VAL	266	56.794	77.170	19.113	1.00	15.56	A	N
ATOM	1932	CA	VAL	266	55.872	76.352	18.347	1.00	12.79	A	C
ATOM	1933	CB	VAL	266	54.856	75.692	19.274	1.00	12.90	A	C
ATOM	1934	CG1	VAL	266	54.193	76.766	20.130	1.00	12.06	A	C
ATOM	1935	CG2	VAL	266	53.821	74.920	18.466	1.00	10.69	A	C
ATOM	1936	C	VAL	266	55.115	77.180	17.350	1.00	12.88	A	C
ATOM	1937	O	VAL	266	54.995	78.388	17.511	1.00	12.12	A	O
ATOM	1938	N	LYS	267	54.601	76.501	16.327	1.00	13.52	A	N
ATOM	1939	CA	LYS	267	53.817	77.107	15.262	1.00	13.08	A	C
ATOM	1940	CB	LYS	267	54.692	77.389	14.050	1.00	13.64	A	C
ATOM	1941	CG	LYS	267	55.642	78.570	14.165	1.00	13.17	A	C
ATOM	1942	CD	LYS	267	56.348	78.713	12.833	1.00	11.33	A	C
ATOM	1943	CE	LYS	267	57.313	79.864	12.788	1.00	11.66	A	C
ATOM	1944	NZ	LYS	267	58.007	79.844	11.459	1.00	12.98	A	N
ATOM	1945	C	LYS	267	52.713	76.136	14.851	1.00	14.81	A	C
ATOM	1946	O	LYS	267	52.885	74.916	14.930	1.00	14.91	A	O
ATOM	1947	N	PHE	268	51.588	76.674	14.389	1.00	15.02	A	N
ATOM	1948	CA	PHE	268	50.471	75.836	13.975	1.00	14.84	A	C
ATOM	1949	CB	PHE	268	49.249	76.138	14.842	1.00	13.98	A	C
ATOM	1950	CG	PHE	268	48.237	75.041	14.846	1.00	15.65	A	C
ATOM	1951	CD1	PHE	268	48.467	73.872	15.562	1.00	15.51	A	C
ATOM	1952	CD2	PHE	268	47.056	75.159	14.115	1.00	18.05	A	C
ATOM	1953	CE1	PHE	268	47.537	72.836	15.551	1.00	15.17	A	C
ATOM	1954	CE2	PHE	268	46.120	74.120	14.101	1.00	17.28	A	C
ATOM	1955	CZ	PHE	268	46.366	72.960	14.821	1.00	14.54	A	C
ATOM	1956	C	PHE	268	50.117	76.029	12.497	1.00	14.63	A	C
ATOM	1957	O	PHE	268	50.143	77.144	11.981	1.00	16.53	A	O
ATOM	1958	N	PHE	269	49.767	74.938	11.829	1.00	13.37	A	N
ATOM	1959	CA	PHE	269	49.417	74.976	10.413	1.00	12.73	A	C

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(Continued)

ATOM	1960	CB	PHE	269	50.597	74.510	9.547	1.00	12.68	A	C
ATOM	1961	CG	PHE	269	51.875	75.229	9.809	1.00	10.71	A	C
ATOM	1962	CD1	PHE	269	52.190	76.387	9.112	1.00	11.11	A	C
ATOM	1963	CD2	PHE	269	52.758	74.759	10.770	1.00	11.04	A	C
ATOM	1964	CE1	PHE	269	53.374	77.070	9.371	1.00	12.54	A	C
ATOM	1965	CE2	PHE	269	53.940	75.430	11.039	1.00	13.96	A	C
ATOM	1966	CZ	PHE	269	54.252	76.591	10.339	1.00	13.89	A	C
ATOM	1967	C	PHE	269	48.270	74.032	10.117	1.00	12.37	A	C
ATOM	1968	O	PHE	269	47.937	73.157	10.910	1.00	14.50	A	O
ATOM	1969	N	VAL	270	47.699	74.193	8.938	1.00	13.63	A	N
ATOM	1970	CA	VAL	270	46.626	73.334	8.485	1.00	15.44	A	C
ATOM	1971	CB	VAL	270	45.228	73.903	8.815	1.00	14.59	A	C
ATOM	1972	CG1	VAL	270	44.153	72.900	8.383	1.00	12.94	A	C
ATOM	1973	CG2	VAL	270	45.110	74.183	10.304	1.00	15.69	A	C
ATOM	1974	C	VAL	270	46.730	73.198	6.975	1.00	16.91	A	C
ATOM	1975	O	VAL	270	46.875	74.188	6.258	1.00	17.51	A	O
ATOM	1976	N	VAL	271	46.681	71.966	6.494	1.00	17.37	A	N
ATOM	1977	CA	VAL	271	46.726	71.746	5.067	1.00	16.54	A	C
ATOM	1978	CB	VAL	271	47.928	70.879	4.646	1.00	19.07	A	C
ATOM	1979	CG1	VAL	271	47.911	69.548	5.400	1.00	20.07	A	C
ATOM	1980	CG2	VAL	271	47.878	70.635	3.131	1.00	18.62	A	C
ATOM	1981	C	VAL	271	45.456	71.041	4.641	1.00	15.09	A	C
ATOM	1982	O	VAL	271	44.912	70.226	5.383	1.00	13.46	A	O
ATOM	1983	N	ASN	272	44.988	71.394	3.449	1.00	15.17	A	N
ATOM	1984	CA	ASN	272	43.812	70.802	2.832	1.00	14.94	A	C
ATOM	1985	CB	ASN	272	43.231	71.767	1.797	1.00	13.83	A	C
ATOM	1986	CG	ASN	272	42.010	71.205	1.093	1.00	14.46	A	C
ATOM	1987	OD1	ASN	272	41.822	69.989	1.007	1.00	16.67	A	O
ATOM	1988	ND2	ASN	272	41.175	72.090	0.581	1.00	15.74	A	N
ATOM	1989	C	ASN	272	44.310	69.542	2.110	1.00	15.70	A	C
ATOM	1990	O	ASN	272	44.755	69.617	0.967	1.00	16.88	A	O
ATOM	1991	N	THR	273	44.241	68.390	2.758	1.00	15.93	A	N
ATOM	1992	CA	THR	273	44.717	67.169	2.124	1.00	18.97	A	C
ATOM	1993	CB	THR	273	44.570	65.936	3.052	1.00	19.44	A	C
ATOM	1994	OG1	THR	273	43.201	65.794	3.471	1.00	19.69	A	O
ATOM	1995	CG2	THR	273	45.481	66.083	4.266	1.00	19.20	A	C
ATOM	1996	C	THR	273	44.009	66.870	0.813	1.00	19.92	A	C
ATOM	1997	O	THR	273	44.550	66.154	-0.028	1.00	21.20	A	O
ATOM	1998	N	ASP	274	42.811	67.424	0.634	1.00	20.50	A	N
ATOM	1999	CA	ASP	274	42.032	67.193	-0.584	1.00	20.30	A	C
ATOM	2000	CB	ASP	274	40.578	67.629	-0.390	1.00	21.02	A	C
ATOM	2001	CG	ASP	274	39.705	66.529	0.178	1.00	23.48	A	C
ATOM	2002	OD1	ASP	274	38.543	66.823	0.527	1.00	26.38	A	O
ATOM	2003	OD2	ASP	274	40.168	65.375	0.275	1.00	23.88	A	O
ATOM	2004	C	ASP	274	42.573	67.870	-1.832	1.00	19.89	A	C
ATOM	2005	O	ASP	274	42.131	67.556	-2.932	1.00	22.08	A	O
ATOM	2006	N	SER	275	43.508	68.802	-1.676	1.00	18.13	A	N
ATOM	2007	CA	SER	275	44.073	69.490	-2.834	1.00	18.83	A	C
ATOM	2008	CB	SER	275	44.284	70.969	-2.518	1.00	19.37	A	C

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(Continued)

## FIG. 4 - 42

ATOM	2009	OG	SER	275	45.197	71.121	-1.444	1.00	24.82	A	O
ATOM	2010	C	SER	275	45.397	68.885	-3.314	1.00	19.53	A	C
ATOM	2011	O	SER	275	45.883	69.226	-4.394	1.00	19.59	A	O
ATOM	2012	N	LEU	276	45.971	67.986	-2.516	1.00	19.83	A	N
ATOM	2013	CA	LEU	276	47.241	67.348	-2.846	1.00	20.72	A	C
ATOM	2014	CB	LEU	276	47.545	66.226	-1.849	1.00	19.96	A	C
ATOM	2015	CG	LEU	276	47.725	66.641	-0.392	1.00	20.47	A	C
ATOM	2016	CD1	LEU	276	47.991	65.410	0.456	1.00	21.68	A	C
ATOM	2017	CD2	LEU	276	48.875	67.622	-0.277	1.00	18.56	A	C
ATOM	2018	C	LEU	276	47.360	66.790	-4.263	1.00	22.34	A	C
ATOM	2019	O	LEU	276	48.290	67.137	-4.994	1.00	24.63	A	O
ATOM	2020	N	SER	277	46.434	65.925	-4.656	1.00	22.80	A	N
ATOM	2021	CA	SER	277	46.501	65.325	-5.983	1.00	23.82	A	C
ATOM	2022	CB	SER	277	45.456	64.219	-6.121	1.00	22.59	A	C
ATOM	2023	OG	SER	277	44.148	64.756	-6.044	1.00	23.44	A	O
ATOM	2024	C	SER	277	46.305	66.341	-7.097	1.00	24.47	A	C
ATOM	2025	O	SER	277	46.699	66.104	-8.231	1.00	26.86	A	O
ATOM	2026	N	SER	278	45.698	67.472	-6.768	1.00	25.44	A	N
ATOM	2027	CA	SER	278	45.431	68.522	-7.745	1.00	26.20	A	C
ATOM	2028	CB	SER	278	44.051	69.121	-7.471	1.00	25.70	A	C
ATOM	2029	OG	SER	278	43.831	70.266	-8.266	1.00	30.53	A	O
ATOM	2030	C	SER	278	46.495	69.630	-7.739	1.00	25.70	A	C
ATOM	2031	O	SER	278	46.603	70.414	-8.683	1.00	23.48	A	O
ATOM	2032	N	VAL	279	47.277	69.692	-6.672	1.00	26.01	A	N
ATOM	2033	CA	VAL	279	48.327	70.696	-6.565	1.00	28.42	A	C
ATOM	2034	CB	VAL	279	48.073	71.634	-5.350	1.00	29.96	A	C
ATOM	2035	CG1	VAL	279	49.372	72.211	-4.834	1.00	32.19	A	C
ATOM	2036	CG2	VAL	279	47.148	72.768	-5.776	1.00	29.00	A	C
ATOM	2037	C	VAL	279	49.704	70.043	-6.470	1.00	28.21	A	C
ATOM	2038	O	VAL	279	49.834	68.872	-6.088	1.00	29.00	A	O
ATOM	2039	N	THR	280	50.728	70.801	-6.848	1.00	26.67	A	N
ATOM	2040	CA	THR	280	52.092	70.306	-6.832	1.00	26.53	A	C
ATOM	2041	CB	THR	280	53.023	71.217	-7.645	1.00	27.22	A	C
ATOM	2042	OG1	THR	280	52.533	71.331	-8.986	1.00	29.98	A	O
ATOM	2043	CG2	THR	280	54.422	70.645	-7.674	1.00	26.85	A	C
ATOM	2044	C	THR	280	52.618	70.254	-5.418	1.00	26.01	A	C
ATOM	2045	O	THR	280	53.184	69.255	-4.986	1.00	27.33	A	O
ATOM	2046	N	ASN	281	52.402	71.341	-4.696	1.00	25.17	A	N
ATOM	2047	CA	ASN	281	52.876	71.474	-3.334	1.00	23.78	A	C
ATOM	2048	CB	ASN	281	54.190	72.250	-3.388	1.00	22.28	A	C
ATOM	2049	CG	ASN	281	54.925	72.287	-2.071	1.00	22.87	A	C
ATOM	2050	OD1	ASN	281	54.603	71.576	-1.116	1.00	20.83	A	O
ATOM	2051	ND2	ASN	281	55.948	73.136	-2.056	1.00	22.18	A	N
ATOM	2052	C	ASN	281	51.818	72.211	-2.506	1.00	23.12	A	C
ATOM	2053	O	ASN	281	51.876	73.431	-2.362	1.00	22.47	A	O
ATOM	2054	N	ALA	282	50.849	71.460	-1.982	1.00	23.33	A	N
ATOM	2055	CA	ALA	282	49.763	72.018	-1.166	1.00	23.40	A	C
ATOM	2056	CB	ALA	282	48.952	70.895	-0.547	1.00	23.19	A	C
ATOM	2057	C	ALA	282	50.320	72.912	-0.071	1.00	24.45	A	C

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(Continued)

## FIG. 4 - 43

ATOM	2058	O	ALA	282	51.180	72.487	0.694	1.00	25.49	A	O
ATOM	2059	N	THR	283	49.817	74.140	0.024	1.00	24.70	A	N
ATOM	2060	CA	THR	283	50.326	75.074	1.021	1.00	25.33	A	C
ATOM	2061	CB	THR	283	50.209	76.540	0.539	1.00	27.36	A	C
ATOM	2062	OG1	THR	283	48.834	76.874	0.353	1.00	29.84	A	O
ATOM	2063	CG2	THR	283	50.947	76.730	-0.785	1.00	30.06	A	C
ATOM	2064	C	THR	283	49.710	74.983	2.406	1.00	24.49	A	C
ATOM	2065	O	THR	283	48.487	74.960	2.578	1.00	24.13	A	O
ATOM	2066	N	SER	284	50.593	74.941	3.396	1.00	23.17	A	N
ATOM	2067	CA	SER	284	50.200	74.872	4.791	1.00	19.88	A	C
ATOM	2068	CB	SER	284	51.317	74.249	5.624	1.00	15.88	A	C
ATOM	2069	OG	SER	284	51.413	72.868	5.350	1.00	14.23	A	O
ATOM	2070	C	SER	284	49.906	76.275	5.288	1.00	19.24	A	C
ATOM	2071	O	SER	284	50.774	77.148	5.253	1.00	18.08	A	O
ATOM	2072	N	ILE	285	48.674	76.478	5.745	1.00	17.36	A	N
ATOM	2073	CA	ILE	285	48.249	77.771	6.242	1.00	16.16	A	C
ATOM	2074	CB	ILE	285	46.754	78.003	5.977	1.00	16.93	A	C
ATOM	2075	CG2	ILE	285	46.384	79.446	6.324	1.00	14.55	A	C
ATOM	2076	CG1	ILE	285	46.434	77.691	4.513	1.00	14.89	A	C
ATOM	2077	CD1	ILE	285	47.230	78.526	3.528	1.00	15.03	A	C
ATOM	2078	C	ILE	285	48.496	77.848	7.733	1.00	16.46	A	C
ATOM	2079	O	ILE	285	48.116	76.963	8.489	1.00	18.69	A	O
ATOM	2080	N	GLN	286	49.130	78.923	8.159	1.00	16.66	A	N
ATOM	2081	CA	GLN	286	49.428	79.088	9.563	1.00	16.43	A	C
ATOM	2082	CB	GLN	286	50.778	79.776	9.717	1.00	16.31	A	C
ATOM	2083	CG	GLN	286	51.184	80.070	11.135	1.00	17.85	A	C
ATOM	2084	CD	GLN	286	52.552	80.713	11.196	1.00	21.44	A	C
ATOM	2085	OE1	GLN	286	53.072	81.005	12.277	1.00	24.09	A	O
ATOM	2086	NE2	GLN	286	53.149	80.939	10.028	1.00	19.13	A	N
ATOM	2087	C	GLN	286	48.360	79.885	10.289	1.00	16.82	A	C
ATOM	2088	O	GLN	286	47.794	80.844	9.754	1.00	17.23	A	O
ATOM	2089	N	ILE	287	48.070	79.453	11.507	1.00	15.99	A	N
ATOM	2090	CA	ILE	287	47.116	80.137	12.355	1.00	15.11	A	C
ATOM	2091	CB	ILE	287	46.036	79.182	12.894	1.00	14.14	A	C
ATOM	2092	CG2	ILE	287	45.147	79.916	13.875	1.00	14.36	A	C
ATOM	2093	CG1	ILE	287	45.206	78.621	11.742	1.00	13.29	A	C
ATOM	2094	CD1	ILE	287	44.111	77.675	12.202	1.00	14.31	A	C
ATOM	2095	C	ILE	287	47.991	80.625	13.506	1.00	15.35	A	C
ATOM	2096	O	ILE	287	48.349	79.860	14.401	1.00	14.39	A	O
ATOM	2097	N	THR	288	48.367	81.894	13.452	1.00	15.01	A	N
ATOM	2098	CA	THR	288	49.215	82.465	14.482	1.00	16.71	A	C
ATOM	2099	CB	THR	288	49.688	83.874	14.093	1.00	17.36	A	C
ATOM	2100	OG1	THR	288	48.548	84.679	13.779	1.00	21.17	A	O
ATOM	2101	CG2	THR	288	50.621	83.813	12.881	1.00	17.64	A	C
ATOM	2102	C	THR	288	48.510	82.553	15.818	1.00	16.02	A	C
ATOM	2103	O	THR	288	47.287	82.668	15.888	1.00	16.28	A	O
ATOM	2104	N	ALA	289	49.301	82.488	16.881	1.00	16.31	A	N
ATOM	2105	CA	ALA	289	48.787	82.582	18.232	1.00	16.67	A	C
ATOM	2106	CB	ALA	289	49.887	82.262	19.207	1.00	18.89	A	C

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(Continued)

## FIG. 4 - 44

ATOM	2107	C	ALA	289	48.280	84.001	18.467	1.00	18.05	A	C
ATOM	2108	O	ALA	289	48.629	84.927	17.733	1.00	19.12	A	O
ATOM	2109	N	PRO	290	47.436	84.193	19.487	1.00	18.60	A	N
ATOM	2110	CD	PRO	290	46.851	83.189	20.388	1.00	18.37	A	C
ATOM	2111	CA	PRO	290	46.906	85.526	19.783	1.00	19.04	A	C
ATOM	2112	CB	PRO	290	45.791	85.234	20.777	1.00	17.58	A	C
ATOM	2113	CG	PRO	290	46.306	84.055	21.499	1.00	19.78	A	C
ATOM	2114	C	PRO	290	47.976	86.447	20.369	1.00	20.45	A	C
ATOM	2115	O	PRO	290	48.866	85.995	21.092	1.00	22.14	A	O
ATOM	2116	N	ALA	291	47.878	87.735	20.054	1.00	19.85	A	N
ATOM	2117	CA	ALA	291	48.829	88.728	20.543	1.00	19.27	A	C
ATOM	2118	CB	ALA	291	48.330	90.132	20.213	1.00	17.30	A	C
ATOM	2119	C	ALA	291	49.101	88.610	22.041	1.00	19.66	A	C
ATOM	2120	O	ALA	291	50.238	88.791	22.489	1.00	21.52	A	O
ATOM	2121	N	SER	292	48.074	88.305	22.825	1.00	19.16	A	N
ATOM	2122	CA	SER	292	48.275	88.185	24.264	1.00	19.97	A	C
ATOM	2123	CB	SER	292	46.936	87.983	24.971	1.00	19.90	A	C
ATOM	2124	OG	SER	292	46.259	86.839	24.487	1.00	24.94	A	O
ATOM	2125	C	SER	292	49.244	87.055	24.618	1.00	20.24	A	C
ATOM	2126	O	SER	292	49.686	86.948	25.760	1.00	21.86	A	O
ATOM	2127	N	MET	293	49.566	86.214	23.635	1.00	20.06	A	N
ATOM	2128	CA	MET	293	50.504	85.104	23.818	1.00	18.78	A	C
ATOM	2129	CB	MET	293	49.987	83.830	23.149	1.00	17.35	A	C
ATOM	2130	CG	MET	293	48.795	83.168	23.797	1.00	15.90	A	C
ATOM	2131	SD	MET	293	49.139	82.503	25.424	1.00	15.89	A	S
ATOM	2132	CE	MET	293	47.655	82.993	26.296	1.00	16.41	A	C
ATOM	2133	C	MET	293	51.831	85.487	23.161	1.00	20.24	A	C
ATOM	2134	O	MET	293	52.912	85.221	23.693	1.00	21.12	A	O
ATOM	2135	N	LEU	294	51.738	86.116	21.995	1.00	20.44	A	N
ATOM	2136	CA	LEU	294	52.918	86.532	21.255	1.00	21.31	A	C
ATOM	2137	CB	LEU	294	52.498	87.104	19.900	1.00	21.19	A	C
ATOM	2138	CG	LEU	294	51.850	86.092	18.944	1.00	23.63	A	C
ATOM	2139	CD1	LEU	294	51.257	86.820	17.747	1.00	22.60	A	C
ATOM	2140	CD2	LEU	294	52.889	85.064	18.493	1.00	20.94	A	C
ATOM	2141	C	LEU	294	53.818	87.533	21.981	1.00	22.05	A	C
ATOM	2142	O	LEU	294	54.953	87.742	21.564	1.00	23.39	A	O
ATOM	2143	N	ILE	295	53.329	88.156	23.053	1.00	21.86	A	N
ATOM	2144	CA	ILE	295	54.149	89.122	23.792	1.00	22.24	A	C
ATOM	2145	CB	ILE	295	53.323	89.938	24.835	1.00	24.92	A	C
ATOM	2146	CG2	ILE	295	52.084	90.536	24.196	1.00	25.08	A	C
ATOM	2147	CG1	ILE	295	52.906	89.034	25.998	1.00	25.57	A	C
ATOM	2148	CD1	ILE	295	52.157	89.761	27.085	1.00	26.45	A	C
ATOM	2149	C	ILE	295	55.271	88.426	24.565	1.00	21.97	A	C
ATOM	2150	O	ILE	295	56.218	89.064	25.006	1.00	23.91	A	O
ATOM	2151	N	GLY	296	55.154	87.119	24.749	1.00	20.65	A	N
ATOM	2152	CA	GLY	296	56.174	86.401	25.482	1.00	18.90	A	C
ATOM	2153	C	GLY	296	56.165	84.922	25.167	1.00	18.45	A	C
ATOM	2154	O	GLY	296	55.527	84.503	24.202	1.00	18.61	A	O
ATOM	2155	N	ASP	297	56.878	84.132	25.967	1.00	16.58	A	N

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ATOM	2156	CA	ASP	297	56.918	82.694	25.751	1.00	16.95	A	C
ATOM	2157	CB	ASP	297	57.960	82.032	26.650	1.00	18.00	A	C
ATOM	2158	CG	ASP	297	59.366	82.378	26.253	1.00	18.62	A	C
ATOM	2159	OD1	ASP	297	59.553	82.882	25.128	1.00	18.23	A	O
ATOM	2160	OD2	ASP	297	60.284	82.134	27.063	1.00	21.29	A	O
ATOM	2161	C	ASP	297	55.553	82.096	26.041	1.00	16.02	A	C
ATOM	2162	O	ASP	297	54.847	82.537	26.942	1.00	16.36	A	O
ATOM	2163	N	HIS	298	55.190	81.079	25.279	1.00	14.79	A	N
ATOM	2164	CA	HIS	298	53.901	80.449	25.460	1.00	16.82	A	C
ATOM	2165	CB	HIS	298	52.846	81.207	24.661	1.00	14.81	A	C
ATOM	2166	CG	HIS	298	53.245	81.448	23.241	1.00	15.31	A	C
ATOM	2167	CD2	HIS	298	52.921	80.793	22.099	1.00	14.85	A	C
ATOM	2168	ND1	HIS	298	54.127	82.442	22.876	1.00	13.01	A	N
ATOM	2169	CE1	HIS	298	54.327	82.392	21.572	1.00	14.39	A	C
ATOM	2170	NE2	HIS	298	53.608	81.400	21.076	1.00	14.38	A	N
ATOM	2171	C	HIS	298	53.956	79.008	24.979	1.00	17.54	A	C
ATOM	2172	O	HIS	298	55.008	78.519	24.560	1.00	15.53	A	O
ATOM	2173	N	TYR	299	52.802	78.348	25.031	1.00	17.25	A	N
ATOM	2174	CA	TYR	299	52.675	76.963	24.609	1.00	16.58	A	C
ATOM	2175	CB	TYR	299	52.666	76.029	25.816	1.00	15.77	A	C
ATOM	2176	CG	TYR	299	53.811	76.176	26.790	1.00	17.03	A	C
ATOM	2177	CD1	TYR	299	55.095	75.762	26.456	1.00	14.29	A	C
ATOM	2178	CE1	TYR	299	56.119	75.807	27.380	1.00	15.79	A	C
ATOM	2179	CD2	TYR	299	53.586	76.653	28.081	1.00	15.17	A	C
ATOM	2180	CE2	TYR	299	54.600	76.700	29.009	1.00	15.67	A	C
ATOM	2181	CZ	TYR	299	55.865	76.270	28.656	1.00	15.90	A	C
ATOM	2182	OH	TYR	299	56.863	76.261	29.595	1.00	16.73	A	O
ATOM	2183	C	TYR	299	51.351	76.741	23.893	1.00	17.76	A	C
ATOM	2184	O	TYR	299	50.349	77.411	24.178	1.00	16.87	A	O
ATOM	2185	N	LEU	300	51.355	75.799	22.959	1.00	16.20	A	N
ATOM	2186	CA	LEU	300	50.130	75.413	22.292	1.00	16.36	A	C
ATOM	2187	CB	LEU	300	50.413	74.923	20.878	1.00	16.40	A	C
ATOM	2188	CG	LEU	300	49.232	74.296	20.139	1.00	14.78	A	C
ATOM	2189	CD1	LEU	300	48.131	75.322	19.972	1.00	16.55	A	C
ATOM	2190	CD2	LEU	300	49.692	73.789	18.785	1.00	15.08	A	C
ATOM	2191	C	LEU	300	49.777	74.243	23.205	1.00	17.58	A	C
ATOM	2192	O	LEU	300	50.568	73.312	23.335	1.00	17.21	A	O
ATOM	2193	N	CYS	301	48.629	74.290	23.873	1.00	19.46	A	N
ATOM	2194	CA	CYS	301	48.288	73.202	24.782	1.00	22.20	A	C
ATOM	2195	CB	CYS	301	48.208	73.722	26.220	1.00	22.63	A	C
ATOM	2196	SG	CYS	301	46.943	74.962	26.503	1.00	26.56	A	S
ATOM	2197	C	CYS	301	47.032	72.399	24.468	1.00	23.29	A	C
ATOM	2198	O	CYS	301	46.690	71.481	25.210	1.00	25.66	A	O
ATOM	2199	N	ASP	302	46.341	72.731	23.386	1.00	23.55	A	N
ATOM	2200	CA	ASP	302	45.148	71.976	23.015	1.00	24.19	A	C
ATOM	2201	CB	ASP	302	43.999	72.223	23.991	1.00	26.49	A	C
ATOM	2202	CG	ASP	302	42.789	71.355	23.680	1.00	28.68	A	C
ATOM	2203	OD1	ASP	302	42.795	70.170	24.066	1.00	30.65	A	O
ATOM	2204	OD2	ASP	302	41.841	71.844	23.029	1.00	30.37	A	O

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(Continued)

## FIG. 4 - 46

ATOM	2205	C	ASP	302	44.658	72.292	21.610	1.00	23.22	A	C
ATOM	2206	O	ASP	302	44.523	73.455	21.226	1.00	24.26	A	O
ATOM	2207	N	VAL	303	44.385	71.237	20.857	1.00	21.65	A	N
ATOM	2208	CA	VAL	303	43.902	71.349	19.493	1.00	20.79	A	C
ATOM	2209	CB	VAL	303	44.926	70.803	18.480	1.00	21.88	A	C
ATOM	2210	CG1	VAL	303	44.420	71.028	17.051	1.00	20.34	A	C
ATOM	2211	CG2	VAL	303	46.273	71.465	18.702	1.00	20.12	A	C
ATOM	2212	C	VAL	303	42.657	70.494	19.417	1.00	20.38	A	C
ATOM	2213	O	VAL	303	42.687	69.306	19.744	1.00	19.45	A	O
ATOM	2214	N	THR	304	41.562	71.102	18.982	1.00	20.04	A	N
ATOM	2215	CA	THR	304	40.302	70.394	18.882	1.00	19.30	A	C
ATOM	2216	CB	THR	304	39.494	70.546	20.191	1.00	19.73	A	C
ATOM	2217	OG1	THR	304	40.256	70.024	21.287	1.00	20.19	A	O
ATOM	2218	CG2	THR	304	38.168	69.812	20.090	1.00	17.51	A	C
ATOM	2219	C	THR	304	39.467	70.930	17.733	1.00	18.56	A	C
ATOM	2220	O	THR	304	39.185	72.127	17.674	1.00	19.32	A	O
ATOM	2221	N	TRP	305	39.082	70.042	16.819	1.00	18.08	A	N
ATOM	2222	CA	TRP	305	38.243	70.422	15.681	1.00	16.88	A	C
ATOM	2223	CB	TRP	305	38.332	69.394	14.546	1.00	13.92	A	C
ATOM	2224	CG	TRP	305	39.581	69.464	13.745	1.00	13.82	A	C
ATOM	2225	CD2	TRP	305	39.815	70.296	12.606	1.00	13.04	A	C
ATOM	2226	CE2	TRP	305	41.143	70.068	12.189	1.00	13.12	A	C
ATOM	2227	CE3	TRP	305	39.031	71.216	11.899	1.00	13.55	A	C
ATOM	2228	CD1	TRP	305	40.745	68.781	13.967	1.00	13.51	A	C
ATOM	2229	NE1	TRP	305	41.688	69.138	13.036	1.00	11.41	A	N
ATOM	2230	CZ2	TRP	305	41.704	70.729	11.094	1.00	12.03	A	C
ATOM	2231	CZ3	TRP	305	39.591	71.873	10.809	1.00	14.16	A	C
ATOM	2232	CH2	TRP	305	40.914	71.625	10.419	1.00	13.92	A	C
ATOM	2233	C	TRP	305	36.803	70.477	16.155	1.00	16.35	A	C
ATOM	2234	O	TRP	305	36.368	69.613	16.917	1.00	16.55	A	O
ATOM	2235	N	ALA	306	36.064	71.484	15.704	1.00	16.10	A	N
ATOM	2236	CA	ALA	306	34.661	71.620	16.079	1.00	17.20	A	C
ATOM	2237	CB	ALA	306	34.336	73.074	16.384	1.00	18.47	A	C
ATOM	2238	C	ALA	306	33.770	71.110	14.956	1.00	16.79	A	C
ATOM	2239	O	ALA	306	32.829	70.369	15.191	1.00	18.46	A	O
ATOM	2240	N	THR	307	34.076	71.516	13.733	1.00	18.36	A	N
ATOM	2241	CA	THR	307	33.314	71.100	12.564	1.00	18.83	A	C
ATOM	2242	CB	THR	307	32.387	72.222	12.072	1.00	18.43	A	C
ATOM	2243	OG1	THR	307	33.178	73.254	11.473	1.00	20.76	A	O
ATOM	2244	CG2	THR	307	31.593	72.811	13.225	1.00	16.72	A	C
ATOM	2245	C	THR	307	34.299	70.778	11.442	1.00	20.34	A	C
ATOM	2246	O	THR	307	35.494	70.626	11.689	1.00	22.05	A	O
ATOM	2247	N	GLN	308	33.798	70.688	10.213	1.00	20.11	A	N
ATOM	2248	CA	GLN	308	34.640	70.389	9.066	1.00	19.71	A	C
ATOM	2249	CB	GLN	308	33.799	69.942	7.866	1.00	19.44	A	C
ATOM	2250	CG	GLN	308	32.845	68.791	8.118	1.00	21.53	A	C
ATOM	2251	CD	GLN	308	33.524	67.505	8.557	1.00	23.81	A	C
ATOM	2252	OE1	GLN	308	32.854	66.565	9.003	1.00	25.80	A	O
ATOM	2253	NE2	GLN	308	34.848	67.449	8.430	1.00	21.04	A	N

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(Continued)

## FIG. 4 - 47

ATOM	2254	C	GLN	308	35.440	71.616	8.653	1.00	19.98	A	C
ATOM	2255	O	GLN	308	36.421	71.501	7.922	1.00	21.84	A	O
ATOM	2256	N	GLU	309	35.022	72.789	9.114	1.00	19.41	A	N
ATOM	2257	CA	GLU	309	35.710	74.019	8.751	1.00	20.93	A	C
ATOM	2258	CB	GLU	309	34.920	74.764	7.685	1.00	21.98	A	C
ATOM	2259	CG	GLU	309	34.709	73.971	6.419	1.00	26.38	A	C
ATOM	2260	CD	GLU	309	33.890	74.731	5.413	1.00	29.11	A	C
ATOM	2261	OE1	GLU	309	33.665	74.192	4.305	1.00	31.98	A	O
ATOM	2262	OE2	GLU	309	33.471	75.869	5.736	1.00	28.78	A	O
ATOM	2263	C	GLU	309	35.924	74.939	9.932	1.00	21.37	A	C
ATOM	2264	O	GLU	309	36.075	76.152	9.764	1.00	21.97	A	O
ATOM	2265	N	ARG	310	35.941	74.360	11.125	1.00	20.65	A	N
ATOM	2266	CA	ARG	310	36.133	75.131	12.340	1.00	20.50	A	C
ATOM	2267	CB	ARG	310	34.779	75.445	12.986	1.00	19.87	A	C
ATOM	2268	CG	ARG	310	34.888	76.186	14.305	1.00	22.38	A	C
ATOM	2269	CD	ARG	310	33.519	76.630	14.786	1.00	21.66	A	C
ATOM	2270	NE	ARG	310	32.952	77.605	13.870	1.00	20.43	A	N
ATOM	2271	CZ	ARG	310	31.660	77.884	13.785	1.00	19.88	A	C
ATOM	2272	NH1	ARG	310	30.794	77.261	14.569	1.00	21.42	A	N
ATOM	2273	NH2	ARG	310	31.235	78.776	12.902	1.00	21.69	A	N
ATOM	2274	C	ARG	310	37.009	74.346	13.304	1.00	19.05	A	C
ATOM	2275	O	ARG	310	36.701	73.214	13.671	1.00	20.19	A	O
ATOM	2276	N	ILE	311	38.108	74.959	13.710	1.00	17.88	A	N
ATOM	2277	CA	ILE	311	39.044	74.320	14.619	1.00	17.41	A	C
ATOM	2278	CB	ILE	311	40.371	73.991	13.859	1.00	17.28	A	C
ATOM	2279	CG2	ILE	311	40.982	75.252	13.305	1.00	14.23	A	C
ATOM	2280	CG1	ILE	311	41.358	73.254	14.765	1.00	17.79	A	C
ATOM	2281	CD1	ILE	311	42.589	72.763	14.011	1.00	15.43	A	C
ATOM	2282	C	ILE	311	39.283	75.258	15.802	1.00	17.03	A	C
ATOM	2283	O	ILE	311	39.267	76.481	15.649	1.00	17.06	A	O
ATOM	2284	N	SER	312	39.461	74.692	16.988	1.00	16.94	A	N
ATOM	2285	CA	SER	312	39.694	75.517	18.163	1.00	18.32	A	C
ATOM	2286	CB	SER	312	38.631	75.244	19.235	1.00	19.09	A	C
ATOM	2287	OG	SER	312	39.008	74.173	20.074	1.00	18.57	A	O
ATOM	2288	C	SER	312	41.084	75.269	18.736	1.00	18.45	A	C
ATOM	2289	O	SER	312	41.552	74.131	18.795	1.00	17.71	A	O
ATOM	2290	N	LEU	313	41.738	76.349	19.148	1.00	19.07	A	N
ATOM	2291	CA	LEU	313	43.080	76.271	19.708	1.00	20.08	A	C
ATOM	2292	CB	LEU	313	44.093	76.931	18.768	1.00	19.12	A	C
ATOM	2293	CG	LEU	313	44.239	76.409	17.341	1.00	20.02	A	C
ATOM	2294	CD1	LEU	313	45.480	77.038	16.712	1.00	19.82	A	C
ATOM	2295	CD2	LEU	313	44.361	74.892	17.351	1.00	20.74	A	C
ATOM	2296	C	LEU	313	43.172	76.957	21.062	1.00	21.08	A	C
ATOM	2297	O	LEU	313	42.608	78.030	21.265	1.00	21.22	A	O
ATOM	2298	N	GLN	314	43.898	76.333	21.981	1.00	22.23	A	N
ATOM	2299	CA	GLN	314	44.096	76.884	23.308	1.00	22.40	A	C
ATOM	2300	CB	GLN	314	43.545	75.935	24.365	1.00	24.62	A	C
ATOM	2301	CG	GLN	314	42.033	75.860	24.406	1.00	27.30	A	C
ATOM	2302	CD	GLN	314	41.536	74.832	25.401	1.00	29.52	A	C

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## FIG. 4 - 48

ATOM	2303	OE1	GLN	314	41.827	74.911	26.598	1.00	29.38	A	O
ATOM	2304	NE2	GLN	314	40.786	73.854	24.911	1.00	30.52	A	N
ATOM	2305	C	GLN	314	45.584	77.099	23.532	1.00	22.00	A	C
ATOM	2306	O	GLN	314	46.382	76.176	23.419	1.00	22.34	A	O
ATOM	2307	N	TRP	315	45.954	78.333	23.833	1.00	21.50	A	N
ATOM	2308	CA	TRP	315	47.343	78.667	24.070	1.00	20.70	A	C
ATOM	2309	CB	TRP	315	47.748	79.873	23.226	1.00	18.74	A	C
ATOM	2310	CG	TRP	315	47.480	79.711	21.746	1.00	17.87	A	C
ATOM	2311	CD2	TRP	315	48.435	79.368	20.733	1.00	14.81	A	C
ATOM	2312	CE2	TRP	315	47.764	79.419	19.491	1.00	14.29	A	C
ATOM	2313	CE3	TRP	315	49.793	79.029	20.753	1.00	13.32	A	C
ATOM	2314	CD1	TRP	315	46.299	79.936	21.095	1.00	15.84	A	C
ATOM	2315	NE1	TRP	315	46.463	79.769	19.742	1.00	13.87	A	N
ATOM	2316	CZ2	TRP	315	48.407	79.147	18.278	1.00	12.51	A	C
ATOM	2317	CZ3	TRP	315	50.433	78.760	19.545	1.00	13.87	A	C
ATOM	2318	CH2	TRP	315	49.736	78.822	18.325	1.00	12.57	A	C
ATOM	2319	C	TRP	315	47.530	78.976	25.545	1.00	21.60	A	C
ATOM	2320	O	TRP	315	46.615	79.463	26.205	1.00	22.41	A	O
ATOM	2321	N	LEU	316	48.721	78.689	26.056	1.00	21.81	A	N
ATOM	2322	CA	LEU	316	49.033	78.915	27.458	1.00	22.64	A	C
ATOM	2323	CB	LEU	316	49.034	77.573	28.192	1.00	22.20	A	C
ATOM	2324	CG	LEU	316	49.655	77.484	29.584	1.00	23.04	A	C
ATOM	2325	CD1	LEU	316	48.953	78.438	30.530	1.00	24.08	A	C
ATOM	2326	CD2	LEU	316	49.557	76.049	30.085	1.00	19.71	A	C
ATOM	2327	C	LEU	316	50.383	79.617	27.618	1.00	24.44	A	C
ATOM	2328	O	LEU	316	51.392	79.192	27.046	1.00	26.77	A	O
ATOM	2329	N	ARG	317	50.388	80.704	28.383	1.00	23.92	A	N
ATOM	2330	CA	ARG	317	51.603	81.475	28.630	1.00	22.55	A	C
ATOM	2331	CB	ARG	317	51.265	82.787	29.337	1.00	25.72	A	C
ATOM	2332	CG	ARG	317	50.490	83.785	28.504	1.00	26.56	A	C
ATOM	2333	CD	ARG	317	50.187	85.012	29.327	1.00	26.99	A	C
ATOM	2334	NE	ARG	317	49.796	86.141	28.494	1.00	30.37	A	N
ATOM	2335	CZ	ARG	317	49.278	87.269	28.966	1.00	30.55	A	C
ATOM	2336	NH1	ARG	317	49.082	87.414	30.273	1.00	29.99	A	N
ATOM	2337	NH2	ARG	317	48.972	88.256	28.132	1.00	28.53	A	N
ATOM	2338	C	ARG	317	52.580	80.705	29.500	1.00	21.07	A	C
ATOM	2339	O	ARG	317	52.175	79.920	30.359	1.00	19.79	A	O
ATOM	2340	N	ARG	318	53.871	80.941	29.290	1.00	19.43	A	N
ATOM	2341	CA	ARG	318	54.876	80.259	30.084	1.00	17.08	A	C
ATOM	2342	CB	ARG	318	56.263	80.850	29.845	1.00	15.15	A	C
ATOM	2343	CG	ARG	318	57.345	80.075	30.564	1.00	13.58	A	C
ATOM	2344	CD	ARG	318	58.671	80.165	29.853	1.00	13.59	A	C
ATOM	2345	NE	ARG	318	59.687	79.341	30.504	1.00	11.13	A	N
ATOM	2346	CZ	ARG	318	60.895	79.135	30.001	1.00	10.46	A	C
ATOM	2347	NH1	ARG	318	61.220	79.694	28.850	1.00	11.29	A	N
ATOM	2348	NH2	ARG	318	61.773	78.378	30.642	1.00	10.86	A	N
ATOM	2349	C	ARG	318	54.500	80.354	31.555	1.00	16.61	A	C
ATOM	2350	O	ARG	318	54.794	79.448	32.318	1.00	20.33	A	O
ATOM	2351	N	ILE	319	53.869	81.455	31.954	1.00	16.59	A	N

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(Continued)

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ATOM	2352	CA	ILE	319	53.396	81.607	33.330	1.00	17.40	A	C
ATOM	2353	CB	ILE	319	53.389	83.078	33.776	1.00	17.03	A	C
ATOM	2354	CG2	ILE	319	52.720	83.210	35.128	1.00	17.19	A	C
ATOM	2355	CG1	ILE	319	54.828	83.589	33.878	1.00	19.57	A	C
ATOM	2356	CD1	ILE	319	55.712	82.743	34.787	1.00	19.56	A	C
ATOM	2357	C	ILE	319	51.972	81.065	33.251	1.00	17.56	A	C
ATOM	2358	O	ILE	319	51.012	81.808	33.067	1.00	18.71	A	O
ATOM	2359	N	GLN	320	51.870	79.747	33.381	1.00	16.94	A	N
ATOM	2360	CA	GLN	320	50.623	79.001	33.246	1.00	16.12	A	C
ATOM	2361	CB	GLN	320	50.939	77.516	33.420	1.00	14.59	A	C
ATOM	2362	CG	GLN	320	52.000	77.044	32.444	1.00	12.17	A	C
ATOM	2363	CD	GLN	320	52.304	75.577	32.570	1.00	10.79	A	C
ATOM	2364	OE1	GLN	320	51.431	74.734	32.403	1.00	12.70	A	O
ATOM	2365	NE2	GLN	320	53.554	75.261	32.860	1.00	13.71	A	N
ATOM	2366	C	GLN	320	49.368	79.351	34.038	1.00	16.32	A	C
ATOM	2367	O	GLN	320	48.645	78.466	34.472	1.00	14.51	A	O
ATOM	2368	N	ASN	321	49.079	80.633	34.207	1.00	18.37	A	N
ATOM	2369	CA	ASN	321	47.871	81.010	34.931	1.00	19.38	A	C
ATOM	2370	CB	ASN	321	48.226	81.785	36.203	1.00	20.21	A	C
ATOM	2371	CG	ASN	321	48.776	83.166	35.925	1.00	23.59	A	C
ATOM	2372	OD1	ASN	321	49.166	83.491	34.804	1.00	22.35	A	O
ATOM	2373	ND2	ASN	321	48.801	83.975	36.980	1.00	27.82	A	N
ATOM	2374	C	ASN	321	46.983	81.843	34.020	1.00	18.69	A	C
ATOM	2375	O	ASN	321	46.095	82.555	34.479	1.00	19.10	A	O
ATOM	2376	N	TYR	322	47.222	81.715	32.719	1.00	17.65	A	N
ATOM	2377	CA	TYR	322	46.482	82.466	31.719	1.00	18.28	A	C
ATOM	2378	CB	TYR	322	47.105	83.856	31.599	1.00	18.09	A	C
ATOM	2379	CG	TYR	322	46.319	84.856	30.792	1.00	20.14	A	C
ATOM	2380	CD1	TYR	322	46.561	85.037	29.428	1.00	21.33	A	C
ATOM	2381	CE1	TYR	322	45.843	85.987	28.694	1.00	22.14	A	C
ATOM	2382	CD2	TYR	322	45.340	85.645	31.401	1.00	20.00	A	C
ATOM	2383	CE2	TYR	322	44.624	86.589	30.681	1.00	19.18	A	C
ATOM	2384	CZ	TYR	322	44.876	86.758	29.334	1.00	21.74	A	C
ATOM	2385	OH	TYR	322	44.163	87.704	28.638	1.00	24.04	A	O
ATOM	2386	C	TYR	322	46.518	81.750	30.363	1.00	18.70	A	C
ATOM	2387	O	TYR	322	47.583	81.587	29.764	1.00	18.36	A	O
ATOM	2388	N	SER	323	45.351	81.318	29.896	1.00	17.43	A	N
ATOM	2389	CA	SER	323	45.237	80.638	28.612	1.00	17.45	A	C
ATOM	2390	CB	SER	323	44.871	79.163	28.806	1.00	16.45	A	C
ATOM	2391	OG	SER	323	43.662	79.025	29.535	1.00	17.51	A	O
ATOM	2392	C	SER	323	44.163	81.320	27.777	1.00	17.88	A	C
ATOM	2393	O	SER	323	43.250	81.943	28.314	1.00	18.20	A	O
ATOM	2394	N	VAL	324	44.277	81.199	26.461	1.00	18.44	A	N
ATOM	2395	CA	VAL	324	43.309	81.802	25.555	1.00	18.83	A	C
ATOM	2396	CB	VAL	324	43.925	82.995	24.800	1.00	19.32	A	C
ATOM	2397	CG1	VAL	324	42.944	83.509	23.760	1.00	18.46	A	C
ATOM	2398	CG2	VAL	324	44.290	84.105	25.785	1.00	18.78	A	C
ATOM	2399	C	VAL	324	42.839	80.776	24.534	1.00	18.47	A	C
ATOM	2400	O	VAL	324	43.631	79.985	24.036	1.00	18.75	A	O

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## FIG. 4 - 50

ATOM	2401	N	MET	325	41.549	80.772	24.231	1.00	17.55	A	N
ATOM	2402	CA	MET	325	41.046	79.832	23.245	1.00	17.68	A	C
ATOM	2403	CB	MET	325	39.832	79.062	23.769	1.00	19.82	A	C
ATOM	2404	CG	MET	325	39.272	78.043	22.774	1.00	20.18	A	C
ATOM	2405	SD	MET	325	37.681	77.304	23.268	1.00	23.11	A	S
ATOM	2406	CE	MET	325	38.209	75.734	23.896	1.00	24.95	A	C
ATOM	2407	C	MET	325	40.641	80.584	21.999	1.00	18.03	A	C
ATOM	2408	O	MET	325	39.932	81.583	22.076	1.00	16.88	A	O
ATOM	2409	N	ASP	326	41.114	80.118	20.852	1.00	18.60	A	N
ATOM	2410	CA	ASP	326	40.749	80.738	19.595	1.00	20.69	A	C
ATOM	2411	CB	ASP	326	41.988	81.158	18.797	1.00	22.43	A	C
ATOM	2412	CG	ASP	326	42.329	82.638	18.970	1.00	26.03	A	C
ATOM	2413	OD1	ASP	326	41.511	83.384	19.547	1.00	26.48	A	O
ATOM	2414	OD2	ASP	326	43.415	83.063	18.518	1.00	28.75	A	O
ATOM	2415	C	ASP	326	39.924	79.739	18.800	1.00	19.88	A	C
ATOM	2416	O	ASP	326	40.254	78.563	18.729	1.00	21.77	A	O
ATOM	2417	N	ILE	327	38.832	80.208	18.223	1.00	20.27	A	N
ATOM	2418	CA	ILE	327	37.980	79.355	17.419	1.00	22.22	A	C
ATOM	2419	CB	ILE	327	36.529	79.393	17.941	1.00	20.50	A	C
ATOM	2420	CG2	ILE	327	35.600	78.697	16.985	1.00	19.07	A	C
ATOM	2421	CG1	ILE	327	36.483	78.691	19.305	1.00	21.51	A	C
ATOM	2422	CD1	ILE	327	35.164	78.766	20.006	1.00	20.97	A	C
ATOM	2423	C	ILE	327	38.113	79.908	16.015	1.00	23.66	A	C
ATOM	2424	O	ILE	327	37.625	80.984	15.716	1.00	26.18	A	O
ATOM	2425	N	CYS	328	38.804	79.162	15.161	1.00	26.09	A	N
ATOM	2426	CA	CYS	328	39.069	79.608	13.805	1.00	26.75	A	C
ATOM	2427	C	CYS	328	38.274	78.890	12.721	1.00	27.13	A	C
ATOM	2428	O	CYS	328	38.168	77.663	12.705	1.00	27.70	A	O
ATOM	2429	CB	CYS	328	40.564	79.481	13.547	1.00	27.02	A	C
ATOM	2430	SG	CYS	328	41.567	79.984	14.986	1.00	28.23	A	S
ATOM	2431	N	ASP	329	37.729	79.686	11.807	1.00	26.60	A	N
ATOM	2432	CA	ASP	329	36.913	79.198	10.710	1.00	26.21	A	C
ATOM	2433	CB	ASP	329	35.595	79.969	10.690	1.00	24.92	A	C
ATOM	2434	CG	ASP	329	34.684	79.595	11.842	1.00	26.75	A	C
ATOM	2435	OD1	ASP	329	35.181	79.407	12.969	1.00	27.44	A	O
ATOM	2436	OD2	ASP	329	33.460	79.493	11.625	1.00	28.96	A	O
ATOM	2437	C	ASP	329	37.613	79.349	9.367	1.00	28.54	A	C
ATOM	2438	O	ASP	329	38.314	80.334	9.120	1.00	29.27	A	O
ATOM	2439	N	TYR	330	37.416	78.371	8.492	1.00	29.31	A	N
ATOM	2440	CA	TYR	330	38.027	78.411	7.173	1.00	29.64	A	C
ATOM	2441	CB	TYR	330	38.011	77.019	6.542	1.00	30.55	A	C
ATOM	2442	CG	TYR	330	38.597	76.980	5.151	1.00	31.78	A	C
ATOM	2443	CD1	TYR	330	39.919	77.367	4.919	1.00	32.26	A	C
ATOM	2444	CE1	TYR	330	40.460	77.341	3.641	1.00	32.18	A	C
ATOM	2445	CD2	TYR	330	37.832	76.561	4.066	1.00	32.94	A	C
ATOM	2446	CE2	TYR	330	38.364	76.526	2.779	1.00	32.62	A	C
ATOM	2447	CZ	TYR	330	39.676	76.920	2.574	1.00	33.67	A	C
ATOM	2448	OH	TYR	330	40.193	76.914	1.299	1.00	34.33	A	O
ATOM	2449	C	TYR	330	37.314	79.387	6.243	1.00	30.14	A	C

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(Continued)

## FIG. 4 - 5 1

ATOM	2450	O	TYR	330	36.098	79.313	6.058	1.00	28.65	A	O
ATOM	2451	N	ASP	331	38.074	80.308	5.666	1.00	31.49	A	N
ATOM	2452	CA	ASP	331	37.511	81.262	4.730	1.00	33.80	A	C
ATOM	2453	CB	ASP	331	38.191	82.618	4.862	1.00	36.63	A	C
ATOM	2454	CG	ASP	331	37.573	83.661	3.956	1.00	39.35	A	C
ATOM	2455	OD1	ASP	331	37.570	83.455	2.724	1.00	40.70	A	O
ATOM	2456	OD2	ASP	331	37.084	84.684	4.479	1.00	42.41	A	O
ATOM	2457	C	ASP	331	37.750	80.696	3.336	1.00	35.29	A	C
ATOM	2458	O	ASP	331	38.865	80.730	2.817	1.00	35.63	A	O
ATOM	2459	N	GLU	332	36.690	80.170	2.743	1.00	36.11	A	N
ATOM	2460	CA	GLU	332	36.755	79.562	1.426	1.00	37.77	A	C
ATOM	2461	CB	GLU	332	35.388	78.970	1.080	1.00	38.87	A	C
ATOM	2462	CG	GLU	332	35.234	78.510	-0.354	1.00	43.60	A	C
ATOM	2463	CD	GLU	332	33.869	77.897	-0.620	1.00	47.15	A	C
ATOM	2464	OE1	GLU	332	33.494	77.771	-1.807	1.00	48.97	A	O
ATOM	2465	OE2	GLU	332	33.175	77.534	0.358	1.00	48.40	A	O
ATOM	2466	C	GLU	332	37.231	80.465	0.293	1.00	38.19	A	C
ATOM	2467	O	GLU	332	37.846	79.982	-0.655	1.00	39.73	A	O
ATOM	2468	N	SER	333	36.968	81.764	0.375	1.00	37.67	A	N
ATOM	2469	CA	SER	333	37.388	82.652	-0.704	1.00	38.09	A	C
ATOM	2470	CB	SER	333	36.445	83.858	-0.814	1.00	38.48	A	C
ATOM	2471	OG	SER	333	36.669	84.795	0.223	1.00	40.60	A	O
ATOM	2472	C	SER	333	38.826	83.135	-0.577	1.00	37.74	A	C
ATOM	2473	O	SER	333	39.324	83.838	-1.448	1.00	38.52	A	O
ATOM	2474	N	SER	334	39.496	82.761	0.506	1.00	38.49	A	N
ATOM	2475	CA	SER	334	40.883	83.163	0.708	1.00	37.49	A	C
ATOM	2476	CB	SER	334	40.995	84.180	1.844	1.00	38.50	A	C
ATOM	2477	OG	SER	334	40.954	83.536	3.108	1.00	38.48	A	O
ATOM	2478	C	SER	334	41.722	81.947	1.058	1.00	35.98	A	C
ATOM	2479	O	SER	334	42.941	82.029	1.148	1.00	36.41	A	O
ATOM	2480	N	GLY	335	41.064	80.817	1.263	1.00	35.13	A	N
ATOM	2481	CA	GLY	335	41.797	79.620	1.620	1.00	35.71	A	C
ATOM	2482	C	GLY	335	42.579	79.872	2.894	1.00	35.19	A	C
ATOM	2483	O	GLY	335	43.574	79.201	3.172	1.00	35.61	A	O
ATOM	2484	N	ARG	336	42.128	80.855	3.666	1.00	33.99	A	N
ATOM	2485	CA	ARG	336	42.783	81.197	4.919	1.00	33.15	A	C
ATOM	2486	CB	ARG	336	43.066	82.696	4.991	1.00	36.78	A	C
ATOM	2487	CG	ARG	336	43.957	83.232	3.884	1.00	42.04	A	C
ATOM	2488	CD	ARG	336	44.807	84.374	4.416	1.00	45.76	A	C
ATOM	2489	NE	ARG	336	44.010	85.359	5.147	1.00	48.92	A	N
ATOM	2490	CZ	ARG	336	44.510	86.192	6.055	1.00	50.76	A	C
ATOM	2491	NH1	ARG	336	45.805	86.159	6.348	1.00	52.08	A	N
ATOM	2492	NH2	ARG	336	43.718	87.057	6.675	1.00	52.33	A	N
ATOM	2493	C	ARG	336	41.935	80.801	6.118	1.00	30.26	A	C
ATOM	2494	O	ARG	336	40.763	80.449	5.981	1.00	29.07	A	O
ATOM	2495	N	TRP	337	42.544	80.869	7.294	1.00	26.94	A	N
ATOM	2496	CA	TRP	337	41.869	80.531	8.533	1.00	24.29	A	C
ATOM	2497	CB	TRP	337	42.616	79.403	9.248	1.00	19.88	A	C
ATOM	2498	CG	TRP	337	42.460	78.074	8.561	1.00	15.10	A	C

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(Continued)

## FIG. 4 - 5 2

ATOM	2499	CD2	TRP	337	41.481	77.077	8.861	1.00	9.80	A	C
ATOM	2500	CE2	TRP	337	41.651	76.026	7.927	1.00	9.92	A	C
ATOM	2501	CE3	TRP	337	40.475	76.970	9.825	1.00	7.74	A	C
ATOM	2502	CD1	TRP	337	43.173	77.601	7.485	1.00	12.90	A	C
ATOM	2503	NE1	TRP	337	42.688	76.369	7.099	1.00	9.82	A	N
ATOM	2504	CZ2	TRP	337	40.849	74.885	7.935	1.00	9.71	A	C
ATOM	2505	CZ3	TRP	337	39.675	75.836	9.832	1.00	7.79	A	C
ATOM	2506	CH2	TRP	337	39.866	74.808	8.894	1.00	10.33	A	C
ATOM	2507	C	TRP	337	41.783	81.758	9.425	1.00	24.55	A	C
ATOM	2508	O	TRP	337	42.794	82.360	9.766	1.00	26.73	A	O
ATOM	2509	N	ASN	338	40.570	82.128	9.806	1.00	25.00	A	N
ATOM	2510	CA	ASN	338	40.381	83.296	10.648	1.00	26.17	A	C
ATOM	2511	CB	ASN	338	39.464	84.300	9.949	1.00	28.44	A	C
ATOM	2512	CG	ASN	338	40.016	84.761	8.612	1.00	30.42	A	C
ATOM	2513	OD1	ASN	338	39.320	84.711	7.596	1.00	32.04	A	O
ATOM	2514	ND2	ASN	338	41.271	85.217	8.606	1.00	28.33	A	N
ATOM	2515	C	ASN	338	39.810	82.958	12.012	1.00	25.29	A	C
ATOM	2516	O	ASN	338	38.957	82.084	12.148	1.00	25.29	A	O
ATOM	2517	N	CYS	339	40.293	83.668	13.023	1.00	25.00	A	N
ATOM	2518	CA	CYS	339	39.833	83.482	14.389	1.00	24.73	A	C
ATOM	2519	C	CYS	339	39.289	84.829	14.888	1.00	22.42	A	C
ATOM	2520	O	CYS	339	40.051	85.717	15.249	1.00	21.56	A	O
ATOM	2521	CB	CYS	339	40.992	83.014	15.285	1.00	25.93	A	C
ATOM	2522	SG	CYS	339	42.199	81.865	14.526	1.00	29.61	A	S
ATOM	2523	N	LEU	340	37.968	84.978	14.889	1.00	22.38	A	N
ATOM	2524	CA	LEU	340	37.333	86.212	15.347	1.00	20.83	A	C
ATOM	2525	CB	LEU	340	35.839	86.185	15.069	1.00	19.89	A	C
ATOM	2526	CG	LEU	340	35.364	86.201	13.626	1.00	19.14	A	C
ATOM	2527	CD1	LEU	340	33.877	85.883	13.593	1.00	19.65	A	C
ATOM	2528	CD2	LEU	340	35.647	87.551	13.012	1.00	19.21	A	C
ATOM	2529	C	LEU	340	37.521	86.406	16.835	1.00	20.16	A	C
ATOM	2530	O	LEU	340	37.337	85.478	17.615	1.00	20.80	A	O
ATOM	2531	N	VAL	341	37.866	87.625	17.225	1.00	20.46	A	N
ATOM	2532	CA	VAL	341	38.066	87.949	18.627	1.00	20.11	A	C
ATOM	2533	CB	VAL	341	38.536	89.399	18.786	1.00	21.45	A	C
ATOM	2534	CG1	VAL	341	38.972	89.647	20.221	1.00	22.38	A	C
ATOM	2535	CG2	VAL	341	39.688	89.672	17.819	1.00	24.28	A	C
ATOM	2536	C	VAL	341	36.770	87.749	19.403	1.00	18.51	A	C
ATOM	2537	O	VAL	341	36.785	87.423	20.585	1.00	17.77	A	O
ATOM	2538	N	ALA	342	35.644	87.941	18.731	1.00	19.68	A	N
ATOM	2539	CA	ALA	342	34.345	87.756	19.370	1.00	19.64	A	C
ATOM	2540	CB	ALA	342	33.228	88.125	18.407	1.00	18.89	A	C
ATOM	2541	C	ALA	342	34.177	86.302	19.829	1.00	19.19	A	C
ATOM	2542	O	ALA	342	33.245	85.987	20.580	1.00	18.12	A	O
ATOM	2543	N	ARG	343	35.078	85.422	19.384	1.00	16.06	A	N
ATOM	2544	CA	ARG	343	35.008	84.017	19.766	1.00	16.37	A	C
ATOM	2545	CB	ARG	343	34.962	83.138	18.521	1.00	18.14	A	C
ATOM	2546	CG	ARG	343	33.726	83.390	17.687	1.00	20.31	A	C
ATOM	2547	CD	ARG	343	33.803	82.695	16.357	1.00	21.82	A	C

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## FIG. 4 - 53

(Continued)

ATOM	2548	NE	ARG	343	32.615	82.969	15.561	1.00	23.94	A	N
ATOM	2549	CZ	ARG	343	32.373	82.415	14.383	1.00	26.14	A	C
ATOM	2550	NH1	ARG	343	33.242	81.559	13.864	1.00	28.42	A	N
ATOM	2551	NH2	ARG	343	31.256	82.703	13.734	1.00	30.23	A	N
ATOM	2552	C	ARG	343	36.164	83.603	20.650	1.00	17.09	A	C
ATOM	2553	O	ARG	343	36.275	82.452	21.057	1.00	16.76	A	O
ATOM	2554	N	GLN	344	37.030	84.553	20.955	1.00	18.05	A	N
ATOM	2555	CA	GLN	344	38.175	84.267	21.791	1.00	18.90	A	C
ATOM	2556	CB	GLN	344	39.191	85.385	21.645	1.00	18.03	A	C
ATOM	2557	CG	GLN	344	40.585	85.012	22.038	1.00	17.99	A	C
ATOM	2558	CD	GLN	344	41.571	86.088	21.657	1.00	18.02	A	C
ATOM	2559	OE1	GLN	344	41.711	87.089	22.353	1.00	17.71	A	O
ATOM	2560	NE2	GLN	344	42.246	85.897	20.527	1.00	17.42	A	N
ATOM	2561	C	GLN	344	37.708	84.170	23.234	1.00	19.61	A	C
ATOM	2562	O	GLN	344	37.069	85.087	23.730	1.00	21.89	A	O
ATOM	2563	N	HIS	345	38.013	83.057	23.897	1.00	18.47	A	N
ATOM	2564	CA	HIS	345	37.624	82.868	25.287	1.00	17.92	A	C
ATOM	2565	CB	HIS	345	36.786	81.600	25.453	1.00	16.07	A	C
ATOM	2566	CG	HIS	345	35.478	81.641	24.726	1.00	15.01	A	C
ATOM	2567	CD2	HIS	345	34.223	81.895	25.164	1.00	14.43	A	C
ATOM	2568	ND1	HIS	345	35.371	81.420	23.369	1.00	15.56	A	N
ATOM	2569	CE1	HIS	345	34.108	81.535	23.002	1.00	12.57	A	C
ATOM	2570	NE2	HIS	345	33.390	81.823	24.073	1.00	14.20	A	N
ATOM	2571	C	HIS	345	38.854	82.789	26.172	1.00	19.64	A	C
ATOM	2572	O	HIS	345	39.839	82.129	25.825	1.00	22.18	A	O
ATOM	2573	N	ILE	346	38.790	83.460	27.319	1.00	20.11	A	N
ATOM	2574	CA	ILE	346	39.899	83.501	28.264	1.00	21.08	A	C
ATOM	2575	CB	ILE	346	40.135	84.928	28.760	1.00	20.44	A	C
ATOM	2576	CG2	ILE	346	41.357	84.972	29.667	1.00	20.95	A	C
ATOM	2577	CG1	ILE	346	40.338	85.860	27.572	1.00	19.87	A	C
ATOM	2578	CD1	ILE	346	40.466	87.298	27.978	1.00	22.20	A	C
ATOM	2579	C	ILE	346	39.657	82.624	29.482	1.00	23.76	A	C
ATOM	2580	O	ILE	346	38.535	82.537	29.975	1.00	24.67	A	O
ATOM	2581	N	GLU	347	40.714	81.976	29.967	1.00	25.01	A	N
ATOM	2582	CA	GLU	347	40.601	81.123	31.141	1.00	28.30	A	C
ATOM	2583	CB	GLU	347	40.459	79.656	30.733	1.00	26.51	A	C
ATOM	2584	CG	GLU	347	40.089	78.740	31.891	1.00	27.38	A	C
ATOM	2585	CD	GLU	347	40.169	77.268	31.527	1.00	29.51	A	C
ATOM	2586	OE1	GLU	347	39.877	76.936	30.359	1.00	29.48	A	O
ATOM	2587	OE2	GLU	347	40.511	76.439	32.405	1.00	29.57	A	O
ATOM	2588	C	GLU	347	41.836	81.288	32.021	1.00	30.87	A	C
ATOM	2589	O	GLU	347	42.865	80.661	31.777	1.00	33.35	A	O
ATOM	2590	N	MET	348	41.741	82.131	33.044	1.00	32.50	A	N
ATOM	2591	CA	MET	348	42.877	82.347	33.926	1.00	34.46	A	C
ATOM	2592	CB	MET	348	43.215	83.843	34.002	1.00	37.48	A	C
ATOM	2593	CG	MET	348	42.168	84.723	34.661	1.00	41.62	A	C
ATOM	2594	SD	MET	348	42.028	86.340	33.825	1.00	48.03	A	S
ATOM	2595	CE	MET	348	43.541	87.158	34.341	1.00	46.60	A	C
ATOM	2596	C	MET	348	42.628	81.784	35.315	1.00	33.55	A	C

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(Continued)

## FIG. 4 - 54

ATOM	2597	O	MET	348	41.656	81.070	35.541	1.00	34.35	A	O
ATOM	2598	N	SER	349	43.534	82.085	36.235	1.00	32.30	A	N
ATOM	2599	CA	SER	349	43.428	81.623	37.612	1.00	31.26	A	C
ATOM	2600	CB	SER	349	43.961	80.197	37.744	1.00	31.22	A	C
ATOM	2601	OG	SER	349	43.912	79.760	39.090	1.00	32.92	A	O
ATOM	2602	C	SER	349	44.244	82.573	38.474	1.00	31.16	A	C
ATOM	2603	O	SER	349	45.355	82.950	38.113	1.00	31.25	A	O
ATOM	2604	N	THR	350	43.682	82.962	39.611	1.00	30.83	A	N
ATOM	2605	CA	THR	350	44.340	83.896	40.516	1.00	28.43	A	C
ATOM	2606	CB	THR	350	43.325	84.938	41.027	1.00	28.93	A	C
ATOM	2607	OG1	THR	350	42.251	84.268	41.703	1.00	27.68	A	O
ATOM	2608	CG2	THR	350	42.751	85.733	39.864	1.00	27.87	A	C
ATOM	2609	C	THR	350	44.971	83.198	41.714	1.00	27.14	A	C
ATOM	2610	O	THR	350	45.781	83.786	42.431	1.00	27.62	A	O
ATOM	2611	N	THR	351	44.610	81.936	41.913	1.00	25.72	A	N
ATOM	2612	CA	THR	351	45.109	81.161	43.035	1.00	24.77	A	C
ATOM	2613	CB	THR	351	43.945	80.536	43.786	1.00	25.52	A	C
ATOM	2614	OG1	THR	351	43.166	79.746	42.877	1.00	24.95	A	O
ATOM	2615	CG2	THR	351	43.069	81.617	44.385	1.00	24.61	A	C
ATOM	2616	C	THR	351	46.081	80.047	42.659	1.00	25.48	A	C
ATOM	2617	O	THR	351	46.648	79.392	43.535	1.00	25.57	A	O
ATOM	2618	N	GLY	352	46.261	79.825	41.361	1.00	25.19	A	N
ATOM	2619	CA	GLY	352	47.170	78.786	40.909	1.00	24.62	A	C
ATOM	2620	C	GLY	352	47.371	78.797	39.403	1.00	24.61	A	C
ATOM	2621	O	GLY	352	47.417	79.853	38.774	1.00	25.15	A	O
ATOM	2622	N	TRP	353	47.499	77.612	38.825	1.00	23.36	A	N
ATOM	2623	CA	TRP	353	47.684	77.470	37.390	1.00	21.38	A	C
ATOM	2624	CB	TRP	353	48.631	76.291	37.116	1.00	17.49	A	C
ATOM	2625	CG	TRP	353	48.272	75.023	37.849	1.00	16.34	A	C
ATOM	2626	CD2	TRP	353	48.587	74.693	39.209	1.00	14.04	A	C
ATOM	2627	CE2	TRP	353	48.053	73.409	39.462	1.00	14.33	A	C
ATOM	2628	CE3	TRP	353	49.270	75.356	40.238	1.00	14.55	A	C
ATOM	2629	CD1	TRP	353	47.578	73.957	37.351	1.00	14.89	A	C
ATOM	2630	NE1	TRP	353	47.445	72.985	38.311	1.00	12.84	A	N
ATOM	2631	CZ2	TRP	353	48.180	72.768	40.709	1.00	14.93	A	C
ATOM	2632	CZ3	TRP	353	49.398	74.719	41.480	1.00	15.27	A	C
ATOM	2633	CH2	TRP	353	48.853	73.436	41.700	1.00	15.07	A	C
ATOM	2634	C	TRP	353	46.303	77.236	36.782	1.00	22.43	A	C
ATOM	2635	O	TRP	353	45.307	77.292	37.495	1.00	22.69	A	O
ATOM	2636	N	VAL	354	46.231	76.990	35.479	1.00	22.83	A	N
ATOM	2637	CA	VAL	354	44.944	76.749	34.836	1.00	24.15	A	C
ATOM	2638	CB	VAL	354	44.818	77.513	33.498	1.00	25.09	A	C
ATOM	2639	CG1	VAL	354	43.610	77.006	32.718	1.00	24.29	A	C
ATOM	2640	CG2	VAL	354	44.673	79.007	33.762	1.00	24.71	A	C
ATOM	2641	C	VAL	354	44.799	75.264	34.569	1.00	24.96	A	C
ATOM	2642	O	VAL	354	45.751	74.628	34.127	1.00	26.10	A	O
ATOM	2643	N	GLY	355	43.609	74.722	34.841	1.00	24.28	A	N
ATOM	2644	CA	GLY	355	43.354	73.303	34.640	1.00	22.67	A	C
ATOM	2645	C	GLY	355	44.040	72.457	35.696	1.00	22.77	A	C

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(Continued)

## FIG. 4 - 55

ATOM	2646	O	GLY	355	44.743	72.989	36.548	1.00	22.56	A	O
ATOM	2647	N	ARG	356	43.843	71.145	35.668	1.00	23.29	A	N
ATOM	2648	CA	ARG	356	44.505	70.299	36.654	1.00	24.86	A	C
ATOM	2649	CB	ARG	356	43.927	68.886	36.645	1.00	24.91	A	C
ATOM	2650	CG	ARG	356	42.495	68.808	37.122	1.00	27.84	A	C
ATOM	2651	CD	ARG	356	41.973	67.391	37.036	1.00	31.58	A	C
ATOM	2652	NE	ARG	356	40.518	67.340	37.149	1.00	35.53	A	N
ATOM	2653	CZ	ARG	356	39.849	67.607	38.261	1.00	37.59	A	C
ATOM	2654	NH1	ARG	356	40.513	67.939	39.362	1.00	40.39	A	N
ATOM	2655	NH2	ARG	356	38.520	67.547	38.272	1.00	37.65	A	N
ATOM	2656	C	ARG	356	45.989	70.255	36.314	1.00	25.60	A	C
ATOM	2657	O	ARG	356	46.844	70.508	37.163	1.00	28.06	A	O
ATOM	2658	N	PHE	357	46.285	69.940	35.060	1.00	23.61	A	N
ATOM	2659	CA	PHE	357	47.659	69.876	34.587	1.00	21.95	A	C
ATOM	2660	CB	PHE	357	48.029	68.442	34.205	1.00	15.99	A	C
ATOM	2661	CG	PHE	357	48.173	67.524	35.380	1.00	12.89	A	C
ATOM	2662	CD1	PHE	357	49.361	67.491	36.115	1.00	11.73	A	C
ATOM	2663	CD2	PHE	357	47.126	66.693	35.763	1.00	10.46	A	C
ATOM	2664	CE1	PHE	357	49.507	66.638	37.216	1.00	7.55	A	C
ATOM	2665	CE2	PHE	357	47.263	65.838	36.863	1.00	11.70	A	C
ATOM	2666	CZ	PHE	357	48.459	65.811	37.591	1.00	6.24	A	C
ATOM	2667	C	PHE	357	47.775	70.786	33.377	1.00	23.17	A	C
ATOM	2668	O	PHE	357	48.877	71.196	33.005	1.00	26.25	A	O
ATOM	2669	N	ARG	358	46.626	71.100	32.782	1.00	20.84	A	N
ATOM	2670	CA	ARG	358	46.541	71.972	31.615	1.00	20.05	A	C
ATOM	2671	CB	ARG	358	47.156	71.297	30.396	1.00	19.30	A	C
ATOM	2672	CG	ARG	358	46.496	69.991	30.011	1.00	21.15	A	C
ATOM	2673	CD	ARG	358	46.866	69.613	28.598	1.00	24.58	A	C
ATOM	2674	NE	ARG	358	46.293	68.333	28.205	1.00	31.68	A	N
ATOM	2675	CZ	ARG	358	46.163	67.924	26.943	1.00	34.22	A	C
ATOM	2676	NH1	ARG	358	46.564	68.701	25.939	1.00	31.56	A	N
ATOM	2677	NH2	ARG	358	45.640	66.727	26.687	1.00	33.62	A	N
ATOM	2678	C	ARG	358	45.081	72.315	31.313	1.00	20.40	A	C
ATOM	2679	O	ARG	358	44.168	71.608	31.734	1.00	20.47	A	O
ATOM	2680	N	PRO	359	44.840	73.404	30.570	1.00	21.33	A	N
ATOM	2681	CD	PRO	359	45.785	74.338	29.940	1.00	20.09	A	C
ATOM	2682	CA	PRO	359	43.455	73.772	30.254	1.00	21.44	A	C
ATOM	2683	CB	PRO	359	43.624	74.911	29.264	1.00	20.76	A	C
ATOM	2684	CG	PRO	359	44.907	75.539	29.713	1.00	21.86	A	C
ATOM	2685	C	PRO	359	42.741	72.574	29.652	1.00	21.94	A	C
ATOM	2686	O	PRO	359	43.314	71.866	28.827	1.00	21.94	A	O
ATOM	2687	N	SER	360	41.499	72.350	30.070	1.00	22.48	A	N
ATOM	2688	CA	SER	360	40.723	71.208	29.596	1.00	24.26	A	C
ATOM	2689	CB	SER	360	39.501	70.986	30.497	1.00	25.29	A	C
ATOM	2690	OG	SER	360	38.505	71.976	30.283	1.00	27.66	A	O
ATOM	2691	C	SER	360	40.262	71.280	28.140	1.00	25.67	A	C
ATOM	2692	O	SER	360	40.117	72.359	27.555	1.00	25.66	A	O
ATOM	2693	N	GLU	361	40.024	70.104	27.573	1.00	25.65	A	N
ATOM	2694	CA	GLU	361	39.581	69.972	26.199	1.00	27.20	A	C

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(Continued)

## FIG. 4 - 5 6

ATOM	2695	CB	GLU	361	39.803	68.540	25.713	1.00	30.37	A	C
ATOM	2696	CG	GLU	361	39.356	67.444	26.683	1.00	36.42	A	C
ATOM	2697	CD	GLU	361	40.340	67.226	27.839	1.00	42.80	A	C
ATOM	2698	OE1	GLU	361	40.317	68.002	28.822	1.00	43.77	A	O
ATOM	2699	OE2	GLU	361	41.152	66.274	27.757	1.00	46.60	A	O
ATOM	2700	C	GLU	361	38.112	70.324	26.052	1.00	25.88	A	C
ATOM	2701	O	GLU	361	37.295	69.955	26.888	1.00	27.12	A	O
ATOM	2702	N	PRO	362	37.760	71.061	24.989	1.00	23.97	A	N
ATOM	2703	CD	PRO	362	38.650	71.837	24.106	1.00	23.33	A	C
ATOM	2704	CA	PRO	362	36.365	71.436	24.767	1.00	22.45	A	C
ATOM	2705	CB	PRO	362	36.485	72.714	23.945	1.00	23.21	A	C
ATOM	2706	CG	PRO	362	37.679	72.437	23.100	1.00	21.08	A	C
ATOM	2707	C	PRO	362	35.621	70.338	24.013	1.00	21.91	A	C
ATOM	2708	O	PRO	362	36.216	69.582	23.249	1.00	22.96	A	O
ATOM	2709	N	HIS	363	34.318	70.259	24.245	1.00	21.59	A	N
ATOM	2710	CA	HIS	363	33.459	69.280	23.596	1.00	19.88	A	C
ATOM	2711	CB	HIS	363	32.868	68.353	24.649	1.00	18.03	A	C
ATOM	2712	CG	HIS	363	33.898	67.568	25.398	1.00	16.56	A	C
ATOM	2713	CD2	HIS	363	34.638	67.880	26.489	1.00	16.19	A	C
ATOM	2714	ND1	HIS	363	34.292	66.303	25.019	1.00	14.56	A	N
ATOM	2715	CE1	HIS	363	35.227	65.869	25.843	1.00	14.60	A	C
ATOM	2716	NE2	HIS	363	35.457	66.808	26.744	1.00	16.65	A	N
ATOM	2717	C	HIS	363	32.364	70.081	22.903	1.00	20.84	A	C
ATOM	2718	O	HIS	363	31.535	70.709	23.564	1.00	20.84	A	O
ATOM	2719	N	PHE	364	32.383	70.075	21.573	1.00	19.87	A	N
ATOM	2720	CA	PHE	364	31.416	70.832	20.786	1.00	18.84	A	C
ATOM	2721	CB	PHE	364	32.042	71.310	19.470	1.00	18.67	A	C
ATOM	2722	CG	PHE	364	33.073	72.390	19.629	1.00	18.84	A	C
ATOM	2723	CD1	PHE	364	34.341	72.096	20.117	1.00	17.51	A	C
ATOM	2724	CD2	PHE	364	32.776	73.708	19.274	1.00	16.76	A	C
ATOM	2725	CE1	PHE	364	35.298	73.095	20.246	1.00	16.92	A	C
ATOM	2726	CE2	PHE	364	33.727	74.711	19.401	1.00	16.24	A	C
ATOM	2727	CZ	PHE	364	34.988	74.404	19.886	1.00	16.59	A	C
ATOM	2728	C	PHE	364	30.172	70.046	20.432	1.00	19.35	A	C
ATOM	2729	O	PHE	364	30.226	68.831	20.262	1.00	20.71	A	O
ATOM	2730	N	THR	365	29.050	70.750	20.313	1.00	18.81	A	N
ATOM	2731	CA	THR	365	27.805	70.113	19.912	1.00	18.11	A	C
ATOM	2732	CB	THR	365	26.600	71.017	20.161	1.00	17.38	A	C
ATOM	2733	OG1	THR	365	26.521	71.991	19.119	1.00	22.40	A	O
ATOM	2734	CG2	THR	365	26.741	71.734	21.487	1.00	13.72	A	C
ATOM	2735	C	THR	365	28.001	69.954	18.409	1.00	17.58	A	C
ATOM	2736	O	THR	365	28.823	70.650	17.824	1.00	16.70	A	O
ATOM	2737	N	LEU	366	27.250	69.058	17.784	1.00	19.74	A	N
ATOM	2738	CA	LEU	366	27.388	68.799	16.350	1.00	19.89	A	C
ATOM	2739	CB	LEU	366	26.237	67.923	15.860	1.00	19.49	A	C
ATOM	2740	CG	LEU	366	26.338	67.381	14.431	1.00	19.63	A	C
ATOM	2741	CD1	LEU	366	27.606	66.542	14.282	1.00	20.45	A	C
ATOM	2742	CD2	LEU	366	25.112	66.539	14.128	1.00	17.80	A	C
ATOM	2743	C	LEU	366	27.503	70.017	15.438	1.00	21.11	A	C

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## FIG. 4 - 5 7

(Continued)

ATOM	2744	O	LEU	366	28.269	69.989	14.476	1.00	24.21	A	O
ATOM	2745	N	ASP	367	26.764	71.084	15.722	1.00	21.26	A	N
ATOM	2746	CA	ASP	367	26.830	72.261	14.867	1.00	22.95	A	C
ATOM	2747	CB	ASP	367	25.567	73.114	15.005	1.00	26.09	A	C
ATOM	2748	CG	ASP	367	25.458	73.796	16.355	1.00	29.82	A	C
ATOM	2749	OD1	ASP	367	26.469	73.849	17.094	1.00	28.76	A	O
ATOM	2750	OD2	ASP	367	24.352	74.296	16.669	1.00	31.88	A	O
ATOM	2751	C	ASP	367	28.047	73.130	15.139	1.00	22.76	A	C
ATOM	2752	O	ASP	367	28.274	74.122	14.448	1.00	25.46	A	O
ATOM	2753	N	GLY	368	28.818	72.772	16.155	1.00	21.02	A	N
ATOM	2754	CA	GLY	368	30.001	73.541	16.480	1.00	18.54	A	C
ATOM	2755	C	GLY	368	29.740	74.946	16.987	1.00	17.42	A	C
ATOM	2756	O	GLY	368	30.678	75.690	17.237	1.00	17.82	A	O
ATOM	2757	N	ASN	369	28.482	75.324	17.164	1.00	17.57	A	N
ATOM	2758	CA	ASN	369	28.196	76.669	17.647	1.00	17.82	A	C
ATOM	2759	CB	ASN	369	26.838	77.129	17.144	1.00	18.92	A	C
ATOM	2760	CG	ASN	369	26.797	77.234	15.649	1.00	22.41	A	C
ATOM	2761	OD1	ASN	369	27.657	77.871	15.038	1.00	23.56	A	O
ATOM	2762	ND2	ASN	369	25.798	76.606	15.038	1.00	26.52	A	N
ATOM	2763	C	ASN	369	28.270	76.838	19.158	1.00	16.27	A	C
ATOM	2764	O	ASN	369	28.185	77.949	19.665	1.00	16.44	A	O
ATOM	2765	N	SER	370	28.432	75.742	19.882	1.00	15.67	A	N
ATOM	2766	CA	SER	370	28.533	75.824	21.330	1.00	16.34	A	C
ATOM	2767	CB	SER	370	27.145	75.766	21.971	1.00	14.45	A	C
ATOM	2768	OG	SER	370	26.523	74.518	21.739	1.00	14.37	A	O
ATOM	2769	C	SER	370	29.381	74.660	21.797	1.00	16.66	A	C
ATOM	2770	O	SER	370	29.565	73.701	21.058	1.00	18.15	A	O
ATOM	2771	N	PHE	371	29.910	74.742	23.014	1.00	17.09	A	N
ATOM	2772	CA	PHE	371	30.735	73.660	23.532	1.00	16.28	A	C
ATOM	2773	CB	PHE	371	32.194	73.808	23.062	1.00	14.83	A	C
ATOM	2774	CG	PHE	371	32.881	75.062	23.546	1.00	11.31	A	C
ATOM	2775	CD1	PHE	371	32.799	76.243	22.818	1.00	11.07	A	C
ATOM	2776	CD2	PHE	371	33.635	75.050	24.726	1.00	11.89	A	C
ATOM	2777	CE1	PHE	371	33.465	77.409	23.256	1.00	12.04	A	C
ATOM	2778	CE2	PHE	371	34.302	76.205	25.178	1.00	9.92	A	C
ATOM	2779	CZ	PHE	371	34.219	77.383	24.444	1.00	9.76	A	C
ATOM	2780	C	PHE	371	30.703	73.545	25.048	1.00	16.26	A	C
ATOM	2781	O	PHE	371	30.362	74.495	25.752	1.00	15.15	A	O
ATOM	2782	N	TYR	372	31.053	72.360	25.536	1.00	16.67	A	N
ATOM	2783	CA	TYR	372	31.091	72.089	26.962	1.00	16.84	A	C
ATOM	2784	CB	TYR	372	30.349	70.801	27.271	1.00	16.79	A	C
ATOM	2785	CG	TYR	372	28.892	70.879	26.914	1.00	18.47	A	C
ATOM	2786	CD1	TYR	372	28.470	70.744	25.589	1.00	16.97	A	C
ATOM	2787	CE1	TYR	372	27.129	70.850	25.255	1.00	19.91	A	C
ATOM	2788	CD2	TYR	372	27.931	71.124	27.901	1.00	18.26	A	C
ATOM	2789	CE2	TYR	372	26.592	71.235	27.581	1.00	19.23	A	C
ATOM	2790	CZ	TYR	372	26.193	71.097	26.258	1.00	21.51	A	C
ATOM	2791	OH	TYR	372	24.860	71.210	25.944	1.00	23.32	A	O
ATOM	2792	C	TYR	372	32.547	71.977	27.367	1.00	18.35	A	C

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(Continued)

## FIG. 4 - 58

ATOM	2793	O	TYR	372	33.388	71.557	26.571	1.00	20.30	A	O
ATOM	2794	N	LYS	373	32.845	72.325	28.611	1.00	18.89	A	N
ATOM	2795	CA	LYS	373	34.224	72.318	29.071	1.00	19.69	A	C
ATOM	2796	CB	LYS	373	34.907	73.541	28.459	1.00	19.69	A	C
ATOM	2797	CG	LYS	373	36.302	73.863	28.889	1.00	20.48	A	C
ATOM	2798	CD	LYS	373	36.658	75.193	28.240	1.00	23.59	A	C
ATOM	2799	CE	LYS	373	38.048	75.703	28.601	1.00	25.15	A	C
ATOM	2800	NZ	LYS	373	38.103	77.196	28.404	1.00	24.26	A	N
ATOM	2801	C	LYS	373	34.277	72.369	30.593	1.00	20.26	A	C
ATOM	2802	O	LYS	373	33.474	73.050	31.231	1.00	21.08	A	O
ATOM	2803	N	ILE	374	35.215	71.634	31.176	1.00	20.43	A	N
ATOM	2804	CA	ILE	374	35.358	71.624	32.621	1.00	19.63	A	C
ATOM	2805	CB	ILE	374	35.960	70.309	33.123	1.00	19.72	A	C
ATOM	2806	CG2	ILE	374	36.100	70.361	34.650	1.00	19.46	A	C
ATOM	2807	CG1	ILE	374	35.095	69.128	32.667	1.00	19.17	A	C
ATOM	2808	CD1	ILE	374	35.652	67.753	33.079	1.00	15.57	A	C
ATOM	2809	C	ILE	374	36.290	72.745	33.046	1.00	19.75	A	C
ATOM	2810	O	ILE	374	37.408	72.846	32.551	1.00	21.23	A	O
ATOM	2811	N	ILE	375	35.824	73.595	33.951	1.00	20.12	A	N
ATOM	2812	CA	ILE	375	36.643	74.684	34.456	1.00	20.15	A	C
ATOM	2813	CB	ILE	375	36.396	76.014	33.700	1.00	20.38	A	C
ATOM	2814	CG2	ILE	375	36.685	75.837	32.215	1.00	20.24	A	C
ATOM	2815	CG1	ILE	375	34.966	76.488	33.919	1.00	20.36	A	C
ATOM	2816	CD1	ILE	375	34.645	77.772	33.186	1.00	21.00	A	C
ATOM	2817	C	ILE	375	36.346	74.893	35.929	1.00	21.63	A	C
ATOM	2818	O	ILE	375	35.283	74.512	36.426	1.00	21.72	A	O
ATOM	2819	N	SER	376	37.301	75.481	36.634	1.00	22.04	A	N
ATOM	2820	CA	SER	376	37.132	75.740	38.051	1.00	23.67	A	C
ATOM	2821	CB	SER	376	38.449	76.228	38.632	1.00	21.76	A	C
ATOM	2822	OG	SER	376	38.336	76.411	40.022	1.00	26.97	A	O
ATOM	2823	C	SER	376	36.063	76.809	38.210	1.00	24.46	A	C
ATOM	2824	O	SER	376	36.042	77.768	37.445	1.00	27.59	A	O
ATOM	2825	N	ASN	377	35.164	76.659	39.177	1.00	25.41	A	N
ATOM	2826	CA	ASN	377	34.128	77.673	39.356	1.00	26.19	A	C
ATOM	2827	CB	ASN	377	32.755	77.023	39.602	1.00	25.06	A	C
ATOM	2828	CG	ASN	377	32.682	76.222	40.894	1.00	22.15	A	C
ATOM	2829	OD1	ASN	377	33.560	76.294	41.750	1.00	23.03	A	O
ATOM	2830	ND2	ASN	377	31.606	75.457	41.039	1.00	20.01	A	N
ATOM	2831	C	ASN	377	34.447	78.685	40.456	1.00	28.48	A	C
ATOM	2832	O	ASN	377	35.574	78.733	40.960	1.00	29.51	A	O
ATOM	2833	N	GLU	378	33.461	79.498	40.822	1.00	30.42	A	N
ATOM	2834	CA	GLU	378	33.659	80.518	41.845	1.00	33.25	A	C
ATOM	2835	CB	GLU	378	32.401	81.390	41.988	1.00	36.97	A	C
ATOM	2836	CG	GLU	378	32.300	82.505	40.939	1.00	44.33	A	C
ATOM	2837	CD	GLU	378	31.099	83.430	41.148	1.00	49.20	A	C
ATOM	2838	OE1	GLU	378	29.946	82.970	40.972	1.00	51.65	A	O
ATOM	2839	OE2	GLU	378	31.312	84.619	41.489	1.00	50.97	A	O
ATOM	2840	C	GLU	378	34.065	79.975	43.208	1.00	32.75	A	C
ATOM	2841	O	GLU	378	34.582	80.718	44.040	1.00	33.80	A	O

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ATOM	2842	N	GLU	379	33.842	78.687	43.436	1.00	31.75	A	N
ATOM	2843	CA	GLU	379	34.192	78.070	44.709	1.00	31.73	A	C
ATOM	2844	CB	GLU	379	33.083	77.141	45.182	1.00	35.37	A	C
ATOM	2845	CG	GLU	379	31.752	77.788	45.416	1.00	40.59	A	C
ATOM	2846	CD	GLU	379	30.678	76.751	45.677	1.00	46.30	A	C
ATOM	2847	OE1	GLU	379	30.363	75.976	44.741	1.00	48.81	A	O
ATOM	2848	OE2	GLU	379	30.159	76.700	46.815	1.00	49.11	A	O
ATOM	2849	C	GLU	379	35.466	77.252	44.589	1.00	30.70	A	C
ATOM	2850	O	GLU	379	35.952	76.712	45.578	1.00	30.56	A	O
ATOM	2851	N	GLY	380	35.986	77.136	43.373	1.00	29.06	A	N
ATOM	2852	CA	GLY	380	37.203	76.377	43.171	1.00	27.19	A	C
ATOM	2853	C	GLY	380	36.979	74.931	42.781	1.00	27.69	A	C
ATOM	2854	O	GLY	380	37.935	74.167	42.662	1.00	27.62	A	O
ATOM	2855	N	TYR	381	35.726	74.540	42.586	1.00	26.46	A	N
ATOM	2856	CA	TYR	381	35.434	73.167	42.191	1.00	26.78	A	C
ATOM	2857	CB	TYR	381	34.175	72.671	42.903	1.00	26.62	A	C
ATOM	2858	CG	TYR	381	34.394	72.448	44.379	1.00	24.99	A	C
ATOM	2859	CD1	TYR	381	34.864	71.225	44.853	1.00	24.93	A	C
ATOM	2860	CE1	TYR	381	35.145	71.035	46.204	1.00	26.71	A	C
ATOM	2861	CD2	TYR	381	34.202	73.486	45.296	1.00	25.27	A	C
ATOM	2862	CE2	TYR	381	34.480	73.312	46.647	1.00	26.88	A	C
ATOM	2863	CZ	TYR	381	34.955	72.082	47.097	1.00	28.08	A	C
ATOM	2864	OH	TYR	381	35.266	71.909	48.429	1.00	28.31	A	O
ATOM	2865	C	TYR	381	35.261	73.100	40.678	1.00	26.94	A	C
ATOM	2866	O	TYR	381	34.542	73.911	40.091	1.00	28.94	A	O
ATOM	2867	N	ARG	382	35.938	72.147	40.045	1.00	24.97	A	N
ATOM	2868	CA	ARG	382	35.855	72.003	38.600	1.00	22.04	A	C
ATOM	2869	CB	ARG	382	37.057	71.211	38.081	1.00	24.10	A	C
ATOM	2870	CG	ARG	382	38.322	72.045	38.110	1.00	24.01	A	C
ATOM	2871	CD	ARG	382	39.606	71.237	38.141	1.00	24.10	A	C
ATOM	2872	NE	ARG	382	40.647	72.083	38.712	1.00	23.35	A	N
ATOM	2873	CZ	ARG	382	41.178	73.132	38.096	1.00	23.31	A	C
ATOM	2874	NH1	ARG	382	40.783	73.449	36.868	1.00	21.52	A	N
ATOM	2875	NH2	ARG	382	42.052	73.907	38.738	1.00	22.46	A	N
ATOM	2876	C	ARG	382	34.548	71.359	38.186	1.00	20.92	A	C
ATOM	2877	O	ARG	382	34.189	70.270	38.645	1.00	18.12	A	O
ATOM	2878	N	HIS	383	33.840	72.068	37.313	1.00	20.45	A	N
ATOM	2879	CA	HIS	383	32.545	71.647	36.813	1.00	20.33	A	C
ATOM	2880	CB	HIS	383	31.440	72.370	37.581	1.00	20.76	A	C
ATOM	2881	CG	HIS	383	31.177	71.797	38.939	1.00	22.34	A	C
ATOM	2882	CD2	HIS	383	31.590	72.189	40.168	1.00	21.75	A	C
ATOM	2883	ND1	HIS	383	30.418	70.661	39.132	1.00	20.42	A	N
ATOM	2884	CE1	HIS	383	30.374	70.380	40.422	1.00	22.91	A	C
ATOM	2885	NE2	HIS	383	31.076	71.291	41.073	1.00	22.25	A	N
ATOM	2886	C	HIS	383	32.404	71.930	35.330	1.00	20.36	A	C
ATOM	2887	O	HIS	383	33.240	72.608	34.728	1.00	19.84	A	O
ATOM	2888	N	ILE	384	31.325	71.420	34.748	1.00	19.26	A	N
ATOM	2889	CA	ILE	384	31.078	71.589	33.329	1.00	17.93	A	C
ATOM	2890	CB	ILE	384	30.232	70.419	32.802	1.00	17.52	A	C

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(Continued)

## FIG. 4 - 60

ATOM	2891	CG2	ILE	384	30.005	70.566	31.290	1.00	15.28	A	C
ATOM	2892	CG1	ILE	384	30.928	69.097	33.155	1.00	12.97	A	C
ATOM	2893	CD1	ILE	384	30.093	67.865	32.909	1.00	9.57	A	C
ATOM	2894	C	ILE	384	30.376	72.898	33.028	1.00	19.30	A	C
ATOM	2895	O	ILE	384	29.333	73.198	33.605	1.00	18.50	A	O
ATOM	2896	N	CYS	385	30.950	73.681	32.120	1.00	21.14	A	N
ATOM	2897	CA	CYS	385	30.349	74.953	31.745	1.00	24.26	A	C
ATOM	2898	C	CYS	385	29.932	74.887	30.284	1.00	23.62	A	C
ATOM	2899	O	CYS	385	30.654	74.334	29.464	1.00	23.61	A	O
ATOM	2900	CB	CYS	385	31.344	76.106	31.958	1.00	27.85	A	C
ATOM	2901	SG	CYS	385	30.561	77.640	32.569	1.00	37.75	A	S
ATOM	2902	N	TYR	386	28.760	75.440	29.973	1.00	23.26	A	N
ATOM	2903	CA	TYR	386	28.237	75.470	28.609	1.00	21.88	A	C
ATOM	2904	CB	TYR	386	26.726	75.271	28.612	1.00	21.89	A	C
ATOM	2905	CG	TYR	386	26.120	75.183	27.228	1.00	23.48	A	C
ATOM	2906	CD1	TYR	386	24.912	75.825	26.930	1.00	23.55	A	C
ATOM	2907	CE1	TYR	386	24.323	75.712	25.665	1.00	24.11	A	C
ATOM	2908	CD2	TYR	386	26.728	74.424	26.223	1.00	22.70	A	C
ATOM	2909	CE2	TYR	386	26.144	74.299	24.956	1.00	23.04	A	C
ATOM	2910	CZ	TYR	386	24.943	74.946	24.686	1.00	24.39	A	C
ATOM	2911	OH	TYR	386	24.358	74.823	23.449	1.00	23.13	A	O
ATOM	2912	C	TYR	386	28.549	76.816	27.962	1.00	22.02	A	C
ATOM	2913	O	TYR	386	28.187	77.868	28.493	1.00	22.52	A	O
ATOM	2914	N	PHE	387	29.201	76.775	26.806	1.00	21.19	A	N
ATOM	2915	CA	PHE	387	29.582	77.988	26.080	1.00	19.95	A	C
ATOM	2916	CB	PHE	387	31.087	77.987	25.781	1.00	17.05	A	C
ATOM	2917	CG	PHE	387	31.970	78.222	26.973	1.00	14.01	A	C
ATOM	2918	CD1	PHE	387	32.547	79.469	27.185	1.00	9.81	A	C
ATOM	2919	CD2	PHE	387	32.293	77.178	27.835	1.00	11.20	A	C
ATOM	2920	CE1	PHE	387	33.440	79.672	28.231	1.00	9.80	A	C
ATOM	2921	CE2	PHE	387	33.185	77.376	28.885	1.00	10.91	A	C
ATOM	2922	CZ	PHE	387	33.762	78.626	29.082	1.00	9.32	A	C
ATOM	2923	C	PHE	387	28.888	78.153	24.727	1.00	20.94	A	C
ATOM	2924	O	PHE	387	28.552	77.180	24.055	1.00	19.77	A	O
ATOM	2925	N	GLN	388	28.706	79.406	24.332	1.00	21.79	A	N
ATOM	2926	CA	GLN	388	28.151	79.742	23.030	1.00	22.21	A	C
ATOM	2927	CB	GLN	388	27.024	80.760	23.177	1.00	23.86	A	C
ATOM	2928	CG	GLN	388	25.745	80.343	22.477	1.00	29.81	A	C
ATOM	2929	CD	GLN	388	25.096	79.126	23.109	1.00	32.86	A	C
ATOM	2930	OE1	GLN	388	24.357	78.391	22.452	1.00	34.98	A	O
ATOM	2931	NE2	GLN	388	25.356	78.913	24.395	1.00	36.34	A	N
ATOM	2932	C	GLN	388	29.403	80.382	22.427	1.00	21.72	A	C
ATOM	2933	O	GLN	388	29.845	81.428	22.893	1.00	22.74	A	O
ATOM	2934	N	ILE	389	29.982	79.745	21.415	1.00	20.66	A	N
ATOM	2935	CA	ILE	389	31.231	80.215	20.821	1.00	21.00	A	C
ATOM	2936	CB	ILE	389	31.466	79.617	19.422	1.00	20.76	A	C
ATOM	2937	CG2	ILE	389	31.410	78.100	19.496	1.00	19.50	A	C
ATOM	2938	CG1	ILE	389	30.448	80.165	18.429	1.00	19.48	A	C
ATOM	2939	CD1	ILE	389	30.813	79.864	16.992	1.00	19.12	A	C

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## FIG. 4 - 6 1

ATOM	2940	C	ILE	389	31.483	81.713	20.735	1.00	23.29	A	C
ATOM	2941	O	ILE	389	32.640	82.146	20.776	1.00	22.48	A	O
ATOM	2942	N	ASP	390	30.423	82.505	20.611	1.00	24.96	A	N
ATOM	2943	CA	ASP	390	30.584	83.953	20.533	1.00	26.49	A	C
ATOM	2944	CB	ASP	390	29.932	84.508	19.275	1.00	29.09	A	C
ATOM	2945	CG	ASP	390	28.467	84.215	19.216	1.00	30.91	A	C
ATOM	2946	OD1	ASP	390	27.754	84.955	18.517	1.00	35.45	A	O
ATOM	2947	OD2	ASP	390	28.029	83.236	19.858	1.00	33.49	A	O
ATOM	2948	C	ASP	390	30.005	84.676	21.738	1.00	26.43	A	C
ATOM	2949	O	ASP	390	29.402	85.735	21.603	1.00	26.54	A	O
ATOM	2950	N	LYS	391	30.163	84.078	22.910	1.00	27.05	A	N
ATOM	2951	CA	LYS	391	29.707	84.679	24.150	1.00	28.81	A	C
ATOM	2952	CB	LYS	391	28.348	84.128	24.566	1.00	28.62	A	C
ATOM	2953	CG	LYS	391	27.203	84.790	23.824	1.00	31.00	A	C
ATOM	2954	CD	LYS	391	25.867	84.228	24.256	1.00	34.06	A	C
ATOM	2955	CE	LYS	391	24.733	84.772	23.413	1.00	33.69	A	C
ATOM	2956	NZ	LYS	391	23.454	84.073	23.742	1.00	36.51	A	N
ATOM	2957	C	LYS	391	30.772	84.369	25.183	1.00	29.11	A	C
ATOM	2958	O	LYS	391	31.192	83.223	25.327	1.00	29.45	A	O
ATOM	2959	N	LYS	392	31.219	85.401	25.888	1.00	29.66	A	N
ATOM	2960	CA	LYS	392	32.281	85.248	26.872	1.00	30.67	A	C
ATOM	2961	CB	LYS	392	33.069	86.558	26.985	1.00	28.28	A	C
ATOM	2962	CG	LYS	392	33.516	87.119	25.636	1.00	27.07	A	C
ATOM	2963	CD	LYS	392	34.330	86.098	24.852	1.00	27.55	A	C
ATOM	2964	CE	LYS	392	34.643	86.588	23.449	1.00	26.02	A	C
ATOM	2965	NZ	LYS	392	35.369	87.872	23.495	1.00	25.63	A	N
ATOM	2966	C	LYS	392	31.824	84.797	28.248	1.00	31.24	A	C
ATOM	2967	O	LYS	392	32.637	84.679	29.162	1.00	32.17	A	O
ATOM	2968	N	ASP	393	30.531	84.548	28.403	1.00	31.57	A	N
ATOM	2969	CA	ASP	393	30.015	84.098	29.690	1.00	33.64	A	C
ATOM	2970	CB	ASP	393	29.052	85.134	30.271	1.00	36.88	A	C
ATOM	2971	CG	ASP	393	29.734	86.450	30.567	1.00	41.66	A	C
ATOM	2972	OD1	ASP	393	30.607	86.475	31.467	1.00	43.84	A	O
ATOM	2973	OD2	ASP	393	29.409	87.455	29.895	1.00	44.39	A	O
ATOM	2974	C	ASP	393	29.309	82.761	29.546	1.00	32.46	A	C
ATOM	2975	O	ASP	393	28.294	82.666	28.859	1.00	32.91	A	O
ATOM	2976	N	CYS	394	29.841	81.731	30.198	1.00	30.05	A	N
ATOM	2977	CA	CYS	394	29.243	80.410	30.115	1.00	28.94	A	C
ATOM	2978	C	CYS	394	28.312	80.116	31.282	1.00	27.56	A	C
ATOM	2979	O	CYS	394	28.262	80.858	32.258	1.00	27.11	A	O
ATOM	2980	CB	CYS	394	30.336	79.338	30.033	1.00	31.03	A	C
ATOM	2981	SG	CYS	394	31.401	79.166	31.504	1.00	34.42	A	S
ATOM	2982	N	THR	395	27.570	79.023	31.167	1.00	25.71	A	N
ATOM	2983	CA	THR	395	26.645	78.608	32.204	1.00	25.01	A	C
ATOM	2984	CB	THR	395	25.208	78.512	31.647	1.00	25.50	A	C
ATOM	2985	OG1	THR	395	24.709	79.833	31.407	1.00	28.36	A	O
ATOM	2986	CG2	THR	395	24.289	77.779	32.620	1.00	21.52	A	C
ATOM	2987	C	THR	395	27.048	77.251	32.772	1.00	24.22	A	C
ATOM	2988	O	THR	395	27.196	76.280	32.036	1.00	24.44	A	O

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(Continued)

## F I G. 4 - 6 2

ATOM	2989	N	PHE	396	27.231	77.185	34.084	1.00	23.09	A	N
ATOM	2990	CA	PHE	396	27.594	75.924	34.715	1.00	23.03	A	C
ATOM	2991	CB	PHE	396	28.138	76.182	36.116	1.00	22.19	A	C
ATOM	2992	CG	PHE	396	29.581	76.617	36.131	1.00	23.20	A	C
ATOM	2993	CD1	PHE	396	30.604	75.697	35.876	1.00	22.48	A	C
ATOM	2994	CD2	PHE	396	29.924	77.935	36.415	1.00	20.97	A	C
ATOM	2995	CE1	PHE	396	31.949	76.086	35.908	1.00	20.26	A	C
ATOM	2996	CE2	PHE	396	31.267	78.331	36.447	1.00	21.70	A	C
ATOM	2997	CZ	PHE	396	32.279	77.400	36.194	1.00	20.27	A	C
ATOM	2998	C	PHE	396	26.373	75.008	34.764	1.00	20.96	A	C
ATOM	2999	O	PHE	396	25.311	75.412	35.218	1.00	20.96	A	O
ATOM	3000	N	ILE	397	26.523	73.779	34.279	1.00	18.88	A	N
ATOM	3001	CA	ILE	397	25.412	72.842	34.262	1.00	18.00	A	C
ATOM	3002	CB	ILE	397	25.266	72.165	32.879	1.00	16.55	A	C
ATOM	3003	CG2	ILE	397	25.350	73.209	31.787	1.00	13.63	A	C
ATOM	3004	CG1	ILE	397	26.366	71.130	32.669	1.00	16.02	A	C
ATOM	3005	CD1	ILE	397	26.180	70.327	31.402	1.00	17.85	A	C
ATOM	3006	C	ILE	397	25.527	71.770	35.338	1.00	19.16	A	C
ATOM	3007	O	ILE	397	24.787	70.787	35.330	1.00	20.44	A	O
ATOM	3008	N	THR	398	26.480	71.956	36.244	1.00	18.55	A	N
ATOM	3009	CA	THR	398	26.681	71.051	37.367	1.00	19.41	A	C
ATOM	3010	CB	THR	398	27.624	69.858	37.051	1.00	19.56	A	C
ATOM	3011	OG1	THR	398	28.978	70.321	36.960	1.00	22.60	A	O
ATOM	3012	CG2	THR	398	27.221	69.178	35.759	1.00	18.50	A	C
ATOM	3013	C	THR	398	27.343	71.899	38.424	1.00	20.24	A	C
ATOM	3014	O	THR	398	27.979	72.903	38.104	1.00	20.11	A	O
ATOM	3015	N	LYS	399	27.185	71.511	39.681	1.00	22.48	A	N
ATOM	3016	CA	LYS	399	27.795	72.258	40.772	1.00	23.72	A	C
ATOM	3017	CB	LYS	399	27.111	73.618	40.941	1.00	24.42	A	C
ATOM	3018	CG	LYS	399	25.689	73.583	41.462	1.00	27.65	A	C
ATOM	3019	CD	LYS	399	25.269	74.996	41.856	1.00	30.77	A	C
ATOM	3020	CE	LYS	399	23.861	75.054	42.414	1.00	31.89	A	C
ATOM	3021	NZ	LYS	399	22.841	74.747	41.377	1.00	35.03	A	N
ATOM	3022	C	LYS	399	27.751	71.476	42.077	1.00	22.46	A	C
ATOM	3023	O	LYS	399	27.125	70.425	42.154	1.00	21.96	A	O
ATOM	3024	N	GLY	400	28.435	71.989	43.093	1.00	21.98	A	N
ATOM	3025	CA	GLY	400	28.463	71.319	44.378	1.00	22.66	A	C
ATOM	3026	C	GLY	400	29.891	71.115	44.839	1.00	24.94	A	C
ATOM	3027	O	GLY	400	30.831	71.449	44.118	1.00	26.10	A	O
ATOM	3028	N	THR	401	30.064	70.566	46.036	1.00	25.34	A	N
ATOM	3029	CA	THR	401	31.400	70.335	46.560	1.00	26.41	A	C
ATOM	3030	CB	THR	401	31.443	70.541	48.095	1.00	27.75	A	C
ATOM	3031	OG1	THR	401	30.615	69.567	48.741	1.00	31.37	A	O
ATOM	3032	CG2	THR	401	30.924	71.927	48.448	1.00	27.06	A	C
ATOM	3033	C	THR	401	31.923	68.945	46.197	1.00	24.83	A	C
ATOM	3034	O	THR	401	32.027	68.049	47.036	1.00	26.74	A	O
ATOM	3035	N	TRP	402	32.229	68.790	44.915	1.00	22.03	A	N
ATOM	3036	CA	TRP	402	32.781	67.569	44.340	1.00	18.83	A	C
ATOM	3037	CB	TRP	402	31.741	66.460	44.268	1.00	16.39	A	C

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(Continued)

ATOM	3038	CG	TRP	402	30.434	66.886	43.709	1.00	17.90	A	C
ATOM	3039	CD2	TRP	402	30.037	66.865	42.332	1.00	19.16	A	C
ATOM	3040	CE2	TRP	402	28.701	67.320	42.278	1.00	20.21	A	C
ATOM	3041	CE3	TRP	402	30.679	66.505	41.137	1.00	18.78	A	C
ATOM	3042	CD1	TRP	402	29.364	67.345	44.409	1.00	17.97	A	C
ATOM	3043	NE1	TRP	402	28.318	67.605	43.562	1.00	20.57	A	N
ATOM	3044	CZ2	TRP	402	27.989	67.425	41.078	1.00	18.32	A	C
ATOM	3045	CZ3	TRP	402	29.972	66.608	39.943	1.00	19.71	A	C
ATOM	3046	CH2	TRP	402	28.637	67.064	39.924	1.00	18.98	A	C
ATOM	3047	C	TRP	402	33.208	67.983	42.944	1.00	18.09	A	C
ATOM	3048	O	TRP	402	32.956	69.117	42.540	1.00	18.12	A	O
ATOM	3049	N	GLU	403	33.831	67.089	42.191	1.00	17.78	A	N
ATOM	3050	CA	GLU	403	34.284	67.484	40.866	1.00	19.48	A	C
ATOM	3051	CB	GLU	403	35.776	67.805	40.926	1.00	20.26	A	C
ATOM	3052	CG	GLU	403	36.122	68.824	41.983	1.00	21.69	A	C
ATOM	3053	CD	GLU	403	37.433	69.522	41.721	1.00	23.95	A	C
ATOM	3054	OE1	GLU	403	37.506	70.728	42.020	1.00	25.27	A	O
ATOM	3055	OE2	GLU	403	38.384	68.880	41.223	1.00	24.57	A	O
ATOM	3056	C	GLU	403	34.028	66.516	39.716	1.00	19.74	A	C
ATOM	3057	O	GLU	403	33.891	65.305	39.916	1.00	20.05	A	O
ATOM	3058	N	VAL	404	33.957	67.073	38.508	1.00	18.47	A	N
ATOM	3059	CA	VAL	404	33.760	66.273	37.305	1.00	17.63	A	C
ATOM	3060	CB	VAL	404	33.070	67.073	36.165	1.00	14.78	A	C
ATOM	3061	CG1	VAL	404	32.974	66.210	34.914	1.00	11.14	A	C
ATOM	3062	CG2	VAL	404	31.683	67.515	36.595	1.00	12.13	A	C
ATOM	3063	C	VAL	404	35.153	65.875	36.836	1.00	18.38	A	C
ATOM	3064	O	VAL	404	35.986	66.732	36.567	1.00	20.01	A	O
ATOM	3065	N	ILE	405	35.410	64.579	36.764	1.00	18.83	A	N
ATOM	3066	CA	ILE	405	36.707	64.088	36.323	1.00	20.05	A	C
ATOM	3067	CB	ILE	405	36.868	62.593	36.653	1.00	21.78	A	C
ATOM	3068	CG2	ILE	405	38.254	62.123	36.283	1.00	16.28	A	C
ATOM	3069	CG1	ILE	405	36.591	62.364	38.146	1.00	24.51	A	C
ATOM	3070	CD1	ILE	405	37.438	63.218	39.079	1.00	26.24	A	C
ATOM	3071	C	ILE	405	36.858	64.290	34.817	1.00	19.94	A	C
ATOM	3072	O	ILE	405	37.912	64.710	34.345	1.00	20.67	A	O
ATOM	3073	N	GLY	406	35.803	63.990	34.064	1.00	19.40	A	N
ATOM	3074	CA	GLY	406	35.869	64.171	32.627	1.00	16.85	A	C
ATOM	3075	C	GLY	406	34.566	63.983	31.881	1.00	16.78	A	C
ATOM	3076	O	GLY	406	33.679	63.268	32.330	1.00	17.43	A	O
ATOM	3077	N	ILE	407	34.459	64.652	30.736	1.00	17.49	A	N
ATOM	3078	CA	ILE	407	33.303	64.569	29.852	1.00	16.98	A	C
ATOM	3079	CB	ILE	407	33.173	65.861	28.998	1.00	16.67	A	C
ATOM	3080	CG2	ILE	407	32.157	65.671	27.874	1.00	16.93	A	C
ATOM	3081	CG1	ILE	407	32.779	67.036	29.895	1.00	16.45	A	C
ATOM	3082	CD1	ILE	407	32.646	68.357	29.157	1.00	11.65	A	C
ATOM	3083	C	ILE	407	33.611	63.392	28.934	1.00	18.17	A	C
ATOM	3084	O	ILE	407	34.599	63.421	28.212	1.00	18.89	A	O
ATOM	3085	N	GLU	408	32.766	62.367	28.945	1.00	20.84	A	N
ATOM	3086	CA	GLU	408	33.000	61.176	28.122	1.00	22.31	A	C

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ATOM	3087	CB	GLU	408	32.691	59.922	28.944	1.00	21.64	A	C
ATOM	3088	CG	GLU	408	33.457	59.860	30.254	1.00	23.48	A	C
ATOM	3089	CD	GLU	408	34.963	59.947	30.048	1.00	26.15	A	C
ATOM	3090	OE1	GLU	408	35.519	59.081	29.337	1.00	28.40	A	O
ATOM	3091	OE2	GLU	408	35.594	60.877	30.596	1.00	25.87	A	O
ATOM	3092	C	GLU	408	32.262	61.097	26.780	1.00	22.35	A	C
ATOM	3093	O	GLU	408	32.743	60.455	25.846	1.00	23.83	A	O
ATOM	3094	N	ALA	409	31.100	61.729	26.671	1.00	22.21	A	N
ATOM	3095	CA	ALA	409	30.356	61.685	25.414	1.00	20.74	A	C
ATOM	3096	CB	ALA	409	29.797	60.294	25.180	1.00	21.17	A	C
ATOM	3097	C	ALA	409	29.235	62.708	25.386	1.00	20.05	A	C
ATOM	3098	O	ALA	409	28.651	63.041	26.413	1.00	19.39	A	O
ATOM	3099	N	LEU	410	28.937	63.201	24.195	1.00	19.25	A	N
ATOM	3100	CA	LEU	410	27.911	64.207	24.038	1.00	19.28	A	C
ATOM	3101	CB	LEU	410	28.559	65.571	23.796	1.00	19.29	A	C
ATOM	3102	CG	LEU	410	27.634	66.778	23.617	1.00	20.83	A	C
ATOM	3103	CD1	LEU	410	26.959	67.089	24.935	1.00	20.92	A	C
ATOM	3104	CD2	LEU	410	28.434	67.987	23.134	1.00	20.28	A	C
ATOM	3105	C	LEU	410	26.998	63.874	22.879	1.00	20.25	A	C
ATOM	3106	O	LEU	410	27.453	63.649	21.758	1.00	20.84	A	O
ATOM	3107	N	THR	411	25.701	63.834	23.150	1.00	19.86	A	N
ATOM	3108	CA	THR	411	24.741	63.561	22.100	1.00	18.40	A	C
ATOM	3109	CB	THR	411	23.902	62.339	22.418	1.00	15.82	A	C
ATOM	3110	OG1	THR	411	23.017	62.649	23.498	1.00	15.79	A	O
ATOM	3111	CG2	THR	411	24.797	61.177	22.811	1.00	14.12	A	C
ATOM	3112	C	THR	411	23.846	64.787	22.050	1.00	20.16	A	C
ATOM	3113	O	THR	411	23.971	65.684	22.882	1.00	21.79	A	O
ATOM	3114	N	SER	412	22.952	64.836	21.074	1.00	20.25	A	N
ATOM	3115	CA	SER	412	22.061	65.972	20.945	1.00	21.09	A	C
ATOM	3116	CB	SER	412	21.206	65.827	19.687	1.00	22.27	A	C
ATOM	3117	OG	SER	412	20.474	64.618	19.721	1.00	25.03	A	O
ATOM	3118	C	SER	412	21.158	66.118	22.153	1.00	21.84	A	C
ATOM	3119	O	SER	412	20.598	67.185	22.379	1.00	22.97	A	O
ATOM	3120	N	ASP	413	21.015	65.054	22.934	1.00	22.56	A	N
ATOM	3121	CA	ASP	413	20.138	65.104	24.097	1.00	24.36	A	C
ATOM	3122	CB	ASP	413	19.036	64.047	23.975	1.00	26.84	A	C
ATOM	3123	CG	ASP	413	18.161	64.243	22.751	1.00	30.28	A	C
ATOM	3124	OD1	ASP	413	17.153	63.515	22.635	1.00	32.47	A	O
ATOM	3125	OD2	ASP	413	18.474	65.111	21.904	1.00	31.81	A	O
ATOM	3126	C	ASP	413	20.822	64.918	25.442	1.00	24.37	A	C
ATOM	3127	O	ASP	413	20.306	65.363	26.470	1.00	25.08	A	O
ATOM	3128	N	TYR	414	21.974	64.259	25.444	1.00	24.23	A	N
ATOM	3129	CA	TYR	414	22.672	63.998	26.694	1.00	23.03	A	C
ATOM	3130	CB	TYR	414	22.369	62.572	27.155	1.00	23.61	A	C
ATOM	3131	CG	TYR	414	20.925	62.332	27.520	1.00	25.79	A	C
ATOM	3132	CD1	TYR	414	20.402	62.822	28.714	1.00	26.31	A	C
ATOM	3133	CE1	TYR	414	19.071	62.621	29.052	1.00	26.99	A	C
ATOM	3134	CD2	TYR	414	20.074	61.629	26.666	1.00	24.67	A	C
ATOM	3135	CE2	TYR	414	18.740	61.424	26.993	1.00	25.53	A	C

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ATOM	3136	CZ	TYR	414	18.246	61.923	28.188	1.00	28.30	A	C
ATOM	3137	OH	TYR	414	16.925	61.731	28.531	1.00	31.69	A	O
ATOM	3138	C	TYR	414	24.180	64.174	26.639	1.00	22.81	A	C
ATOM	3139	O	TYR	414	24.811	64.040	25.582	1.00	22.74	A	O
ATOM	3140	N	LEU	415	24.741	64.469	27.809	1.00	20.51	A	N
ATOM	3141	CA	LEU	415	26.174	64.630	27.996	1.00	18.28	A	C
ATOM	3142	CB	LEU	415	26.502	66.079	28.358	1.00	16.58	A	C
ATOM	3143	CG	LEU	415	27.945	66.406	28.745	1.00	14.79	A	C
ATOM	3144	CD1	LEU	415	28.184	67.892	28.606	1.00	13.01	A	C
ATOM	3145	CD2	LEU	415	28.208	65.943	30.163	1.00	14.04	A	C
ATOM	3146	C	LEU	415	26.518	63.684	29.149	1.00	18.57	A	C
ATOM	3147	O	LEU	415	25.926	63.763	30.230	1.00	18.31	A	O
ATOM	3148	N	TYR	416	27.449	62.769	28.909	1.00	19.11	A	N
ATOM	3149	CA	TYR	416	27.843	61.796	29.924	1.00	19.69	A	C
ATOM	3150	CB	TYR	416	27.963	60.407	29.309	1.00	18.66	A	C
ATOM	3151	CG	TYR	416	26.698	59.926	28.645	1.00	17.78	A	C
ATOM	3152	CD1	TYR	416	26.297	60.438	27.410	1.00	16.67	A	C
ATOM	3153	CE1	TYR	416	25.137	59.971	26.786	1.00	18.58	A	C
ATOM	3154	CD2	TYR	416	25.908	58.944	29.245	1.00	16.22	A	C
ATOM	3155	CE2	TYR	416	24.754	58.475	28.636	1.00	16.35	A	C
ATOM	3156	CZ	TYR	416	24.374	58.986	27.406	1.00	18.54	A	C
ATOM	3157	OH	TYR	416	23.252	58.489	26.784	1.00	19.53	A	O
ATOM	3158	C	TYR	416	29.167	62.178	30.540	1.00	20.71	A	C
ATOM	3159	O	TYR	416	30.117	62.499	29.822	1.00	22.92	A	O
ATOM	3160	N	TYR	417	29.238	62.138	31.866	1.00	19.27	A	N
ATOM	3161	CA	TYR	417	30.472	62.506	32.544	1.00	19.08	A	C
ATOM	3162	CB	TYR	417	30.408	63.981	32.970	1.00	18.38	A	C
ATOM	3163	CG	TYR	417	29.383	64.282	34.049	1.00	17.93	A	C
ATOM	3164	CD1	TYR	417	29.721	64.213	35.399	1.00	15.25	A	C
ATOM	3165	CE1	TYR	417	28.784	64.476	36.391	1.00	13.14	A	C
ATOM	3166	CD2	TYR	417	28.071	64.622	33.718	1.00	17.72	A	C
ATOM	3167	CE2	TYR	417	27.120	64.885	34.710	1.00	15.27	A	C
ATOM	3168	CZ	TYR	417	27.488	64.808	36.040	1.00	14.25	A	C
ATOM	3169	OH	TYR	417	26.556	65.046	37.020	1.00	14.06	A	O
ATOM	3170	C	TYR	417	30.768	61.615	33.747	1.00	18.77	A	C
ATOM	3171	O	TYR	417	29.918	60.853	34.207	1.00	18.74	A	O
ATOM	3172	N	ILE	418	31.996	61.706	34.236	1.00	17.63	A	N
ATOM	3173	CA	ILE	418	32.429	60.926	35.379	1.00	16.60	A	C
ATOM	3174	CB	ILE	418	33.626	60.019	35.015	1.00	15.54	A	C
ATOM	3175	CG2	ILE	418	34.482	59.737	36.241	1.00	14.33	A	C
ATOM	3176	CG1	ILE	418	33.107	58.729	34.378	1.00	15.75	A	C
ATOM	3177	CD1	ILE	418	34.183	57.767	33.964	1.00	15.48	A	C
ATOM	3178	C	ILE	418	32.827	61.909	36.453	1.00	18.54	A	C
ATOM	3179	O	ILE	418	33.535	62.875	36.190	1.00	20.83	A	O
ATOM	3180	N	SER	419	32.356	61.671	37.664	1.00	19.59	A	N
ATOM	3181	CA	SER	419	32.670	62.556	38.764	1.00	20.34	A	C
ATOM	3182	CB	SER	419	31.523	63.526	38.996	1.00	21.79	A	C
ATOM	3183	OG	SER	419	30.415	62.843	39.562	1.00	24.33	A	O
ATOM	3184	C	SER	419	32.875	61.732	40.013	1.00	20.37	A	C

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ATOM	3185	O	SER	419	32.783	60.503	39.988	1.00	20.32	A	O
ATOM	3186	N	ASN	420	33.152	62.427	41.107	1.00	19.64	A	N
ATOM	3187	CA	ASN	420	33.357	61.786	42.387	1.00	20.07	A	C
ATOM	3188	CB	ASN	420	34.773	62.053	42.863	1.00	18.49	A	C
ATOM	3189	CG	ASN	420	35.099	63.518	42.872	1.00	20.69	A	C
ATOM	3190	OD1	ASN	420	34.210	64.358	42.741	1.00	21.49	A	O
ATOM	3191	ND2	ASN	420	36.376	63.844	43.034	1.00	21.39	A	N
ATOM	3192	C	ASN	420	32.350	62.368	43.379	1.00	20.90	A	C
ATOM	3193	O	ASN	420	32.677	62.610	44.535	1.00	21.17	A	O
ATOM	3194	N	GLU	421	31.127	62.600	42.914	1.00	21.68	A	N
ATOM	3195	CA	GLU	421	30.081	63.160	43.761	1.00	24.26	A	C
ATOM	3196	CB	GLU	421	28.935	63.722	42.901	1.00	26.18	A	C
ATOM	3197	CG	GLU	421	27.714	64.214	43.701	1.00	25.32	A	C
ATOM	3198	CD	GLU	421	26.604	64.817	42.824	1.00	26.09	A	C
ATOM	3199	OE1	GLU	421	25.563	65.237	43.373	1.00	24.11	A	O
ATOM	3200	OE2	GLU	421	26.762	64.873	41.588	1.00	27.22	A	O
ATOM	3201	C	GLU	421	29.512	62.133	44.729	1.00	24.93	A	C
ATOM	3202	O	GLU	421	29.185	62.457	45.868	1.00	27.30	A	O
ATOM	3203	N	TYR	422	29.409	60.892	44.272	1.00	23.63	A	N
ATOM	3204	CA	TYR	422	28.837	59.826	45.075	1.00	23.67	A	C
ATOM	3205	CB	TYR	422	28.942	58.503	44.311	1.00	23.61	A	C
ATOM	3206	CG	TYR	422	28.015	57.415	44.813	1.00	24.39	A	C
ATOM	3207	CD1	TYR	422	26.642	57.637	44.936	1.00	23.87	A	C
ATOM	3208	CE1	TYR	422	25.781	56.618	45.347	1.00	22.11	A	C
ATOM	3209	CD2	TYR	422	28.505	56.147	45.120	1.00	24.53	A	C
ATOM	3210	CE2	TYR	422	27.654	55.124	45.533	1.00	23.32	A	C
ATOM	3211	CZ	TYR	422	26.300	55.367	45.641	1.00	23.52	A	C
ATOM	3212	OH	TYR	422	25.471	54.349	46.031	1.00	24.33	A	O
ATOM	3213	C	TYR	422	29.399	59.679	46.493	1.00	23.57	A	C
ATOM	3214	O	TYR	422	30.599	59.478	46.704	1.00	23.17	A	O
ATOM	3215	N	LYS	423	28.492	59.784	47.461	1.00	23.07	A	N
ATOM	3216	CA	LYS	423	28.813	59.661	48.878	1.00	22.04	A	C
ATOM	3217	CB	LYS	423	29.156	58.205	49.205	1.00	24.22	A	C
ATOM	3218	CG	LYS	423	27.967	57.266	49.009	1.00	25.11	A	C
ATOM	3219	CD	LYS	423	28.303	55.809	49.276	1.00	26.55	A	C
ATOM	3220	CE	LYS	423	27.079	54.930	49.002	1.00	28.11	A	C
ATOM	3221	NZ	LYS	423	27.302	53.498	49.336	1.00	27.79	A	N
ATOM	3222	C	LYS	423	29.923	60.583	49.347	1.00	21.46	A	C
ATOM	3223	O	LYS	423	30.533	60.340	50.385	1.00	20.97	A	O
ATOM	3224	N	GLY	424	30.167	61.647	48.583	1.00	21.39	A	N
ATOM	3225	CA	GLY	424	31.201	62.608	48.930	1.00	21.20	A	C
ATOM	3226	C	GLY	424	32.606	62.034	48.961	1.00	21.98	A	C
ATOM	3227	O	GLY	424	33.463	62.534	49.687	1.00	22.19	A	O
ATOM	3228	N	MET	425	32.848	60.991	48.173	1.00	22.44	A	N
ATOM	3229	CA	MET	425	34.161	60.350	48.134	1.00	23.29	A	C
ATOM	3230	CB	MET	425	34.003	58.826	48.056	1.00	24.14	A	C
ATOM	3231	CG	MET	425	33.548	58.187	49.360	1.00	25.32	A	C
ATOM	3232	SD	MET	425	33.092	56.451	49.179	1.00	29.39	A	S
ATOM	3233	CE	MET	425	34.663	55.611	49.406	1.00	27.92	A	C

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ATOM	3234	C	MET	425	35.042	60.827	46.986	1.00	22.06	A	C
ATOM	3235	O	MET	425	34.836	60.457	45.835	1.00	22.61	A	O
ATOM	3236	N	PRO	426	36.045	61.661	47.292	1.00	21.75	A	N
ATOM	3237	CD	PRO	426	36.386	62.215	48.615	1.00	21.34	A	C
ATOM	3238	CA	PRO	426	36.951	62.172	46.262	1.00	20.07	A	C
ATOM	3239	CB	PRO	426	37.943	63.007	47.062	1.00	20.22	A	C
ATOM	3240	CG	PRO	426	37.138	63.461	48.245	1.00	19.61	A	C
ATOM	3241	C	PRO	426	37.636	61.019	45.532	1.00	20.63	A	C
ATOM	3242	O	PRO	426	37.920	61.107	44.343	1.00	23.99	A	O
ATOM	3243	N	GLY	427	37.905	59.936	46.252	1.00	19.08	A	N
ATOM	3244	CA	GLY	427	38.552	58.789	45.646	1.00	18.03	A	C
ATOM	3245	C	GLY	427	37.601	57.838	44.941	1.00	18.93	A	C
ATOM	3246	O	GLY	427	37.965	56.706	44.642	1.00	21.55	A	O
ATOM	3247	N	GLY	428	36.378	58.285	44.684	1.00	18.22	A	N
ATOM	3248	CA	GLY	428	35.417	57.446	43.991	1.00	17.96	A	C
ATOM	3249	C	GLY	428	35.208	57.970	42.583	1.00	18.15	A	C
ATOM	3250	O	GLY	428	35.577	59.108	42.289	1.00	19.00	A	O
ATOM	3251	N	ARG	429	34.619	57.158	41.712	1.00	16.78	A	N
ATOM	3252	CA	ARG	429	34.389	57.559	40.320	1.00	17.38	A	C
ATOM	3253	CB	ARG	429	35.595	57.167	39.444	1.00	19.09	A	C
ATOM	3254	CG	ARG	429	36.577	58.292	39.108	1.00	20.57	A	C
ATOM	3255	CD	ARG	429	37.385	58.737	40.302	1.00	22.65	A	C
ATOM	3256	NE	ARG	429	38.359	59.769	39.956	1.00	25.75	A	N
ATOM	3257	CZ	ARG	429	39.078	60.445	40.852	1.00	26.83	A	C
ATOM	3258	NH1	ARG	429	38.927	60.204	42.146	1.00	26.78	A	N
ATOM	3259	NH2	ARG	429	39.957	61.356	40.456	1.00	26.24	A	N
ATOM	3260	C	ARG	429	33.134	56.889	39.756	1.00	15.74	A	C
ATOM	3261	O	ARG	429	32.976	55.675	39.857	1.00	12.14	A	O
ATOM	3262	N	ASN	430	32.256	57.679	39.146	1.00	14.98	A	N
ATOM	3263	CA	ASN	430	31.027	57.136	38.586	1.00	17.41	A	C
ATOM	3264	CB	ASN	430	29.901	57.216	39.622	1.00	17.29	A	C
ATOM	3265	CG	ASN	430	29.947	56.081	40.620	1.00	18.53	A	C
ATOM	3266	OD1	ASN	430	29.607	54.938	40.297	1.00	16.68	A	O
ATOM	3267	ND2	ASN	430	30.381	56.386	41.840	1.00	15.65	A	N
ATOM	3268	C	ASN	430	30.564	57.808	37.297	1.00	17.98	A	C
ATOM	3269	O	ASN	430	30.849	58.976	37.043	1.00	19.64	A	O
ATOM	3270	N	LEU	431	29.840	57.053	36.485	1.00	17.00	A	N
ATOM	3271	CA	LEU	431	29.314	57.576	35.241	1.00	17.70	A	C
ATOM	3272	CB	LEU	431	29.122	56.442	34.231	1.00	15.35	A	C
ATOM	3273	CG	LEU	431	28.478	56.867	32.913	1.00	15.33	A	C
ATOM	3274	CD1	LEU	431	29.340	57.917	32.230	1.00	13.77	A	C
ATOM	3275	CD2	LEU	431	28.296	55.645	32.018	1.00	17.37	A	C
ATOM	3276	C	LEU	431	27.978	58.279	35.491	1.00	19.03	A	C
ATOM	3277	O	LEU	431	27.095	57.750	36.172	1.00	17.62	A	O
ATOM	3278	N	TYR	432	27.840	59.475	34.933	1.00	20.33	A	N
ATOM	3279	CA	TYR	432	26.620	60.248	35.083	1.00	21.23	A	C
ATOM	3280	CB	TYR	432	26.848	61.442	36.014	1.00	22.85	A	C
ATOM	3281	CG	TYR	432	27.068	61.070	37.464	1.00	25.34	A	C
ATOM	3282	CD1	TYR	432	28.320	60.646	37.921	1.00	24.87	A	C

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## FIG. 4 - 68

(Continued)

ATOM	3283	CE1	TYR	432	28.519	60.305	39.267	1.00	24.97	A	C
ATOM	3284	CD2	TYR	432	26.019	61.142	38.384	1.00	24.85	A	C
ATOM	3285	CE2	TYR	432	26.205	60.805	39.723	1.00	25.31	A	C
ATOM	3286	CZ	TYR	432	27.454	60.388	40.161	1.00	25.88	A	C
ATOM	3287	OH	TYR	432	27.625	60.054	41.487	1.00	25.59	A	O
ATOM	3288	C	TYR	432	26.102	60.743	33.737	1.00	21.26	A	C
ATOM	3289	O	TYR	432	26.860	60.870	32.770	1.00	21.07	A	O
ATOM	3290	N	LYS	433	24.802	61.022	33.695	1.00	20.78	A	N
ATOM	3291	CA	LYS	433	24.133	61.505	32.496	1.00	20.98	A	C
ATOM	3292	CB	LYS	433	23.290	60.386	31.876	1.00	21.14	A	C
ATOM	3293	CG	LYS	433	22.564	60.827	30.618	1.00	25.64	A	C
ATOM	3294	CD	LYS	433	21.843	59.701	29.907	1.00	25.30	A	C
ATOM	3295	CE	LYS	433	20.643	59.235	30.682	1.00	25.25	A	C
ATOM	3296	NZ	LYS	433	19.801	58.370	29.817	1.00	27.99	A	N
ATOM	3297	C	LYS	433	23.228	62.687	32.835	1.00	20.46	A	C
ATOM	3298	O	LYS	433	22.367	62.587	33.707	1.00	21.41	A	O
ATOM	3299	N	ILE	434	23.427	63.812	32.162	1.00	20.15	A	N
ATOM	3300	CA	ILE	434	22.591	64.980	32.417	1.00	21.18	A	C
ATOM	3301	CB	ILE	434	23.427	66.225	32.815	1.00	21.51	A	C
ATOM	3302	CG2	ILE	434	24.412	66.582	31.715	1.00	22.39	A	C
ATOM	3303	CG1	ILE	434	22.491	67.404	33.083	1.00	22.04	A	C
ATOM	3304	CD1	ILE	434	23.171	68.591	33.699	1.00	23.38	A	C
ATOM	3305	C	ILE	434	21.782	65.297	31.174	1.00	20.81	A	C
ATOM	3306	O	ILE	434	22.274	65.154	30.056	1.00	21.15	A	O
ATOM	3307	N	GLN	435	20.538	65.716	31.372	1.00	21.40	A	N
ATOM	3308	CA	GLN	435	19.666	66.034	30.248	1.00	23.73	A	C
ATOM	3309	CB	GLN	435	18.202	65.851	30.646	1.00	26.08	A	C
ATOM	3310	CG	GLN	435	17.227	66.030	29.496	1.00	29.99	A	C
ATOM	3311	CD	GLN	435	15.802	65.806	29.929	1.00	32.10	A	C
ATOM	3312	OE1	GLN	435	15.446	64.720	30.372	1.00	34.41	A	O
ATOM	3313	NE2	GLN	435	14.978	66.839	29.819	1.00	34.05	A	N
ATOM	3314	C	GLN	435	19.891	67.450	29.743	1.00	22.81	A	C
ATOM	3315	O	GLN	435	19.600	68.419	30.434	1.00	22.20	A	O
ATOM	3316	N	LEU	436	20.401	67.564	28.524	1.00	23.57	A	N
ATOM	3317	CA	LEU	436	20.679	68.865	27.951	1.00	24.55	A	C
ATOM	3318	CB	LEU	436	21.152	68.714	26.508	1.00	21.18	A	C
ATOM	3319	CG	LEU	436	22.456	67.939	26.332	1.00	21.36	A	C
ATOM	3320	CD1	LEU	436	22.938	68.116	24.910	1.00	20.02	A	C
ATOM	3321	CD2	LEU	436	23.510	68.437	27.317	1.00	19.70	A	C
ATOM	3322	C	LEU	436	19.491	69.812	28.020	1.00	26.85	A	C
ATOM	3323	O	LEU	436	19.672	71.016	28.168	1.00	28.66	A	O
ATOM	3324	N	SER	437	18.280	69.268	27.927	1.00	30.22	A	N
ATOM	3325	CA	SER	437	17.059	70.075	27.977	1.00	32.38	A	C
ATOM	3326	CB	SER	437	15.925	69.340	27.268	1.00	32.98	A	C
ATOM	3327	OG	SER	437	16.241	69.151	25.901	1.00	39.22	A	O
ATOM	3328	C	SER	437	16.610	70.437	29.394	1.00	33.81	A	C
ATOM	3329	O	SER	437	15.805	71.352	29.577	1.00	32.20	A	O
ATOM	3330	N	ASP	438	17.124	69.714	30.387	1.00	35.36	A	N
ATOM	3331	CA	ASP	438	16.772	69.955	31.784	1.00	36.00	A	C

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## FIG. 4 - 69

(Continued)

ATOM	3332	CB	ASP	438	15.468	69.226	32.123	1.00	38.49	A	C
ATOM	3333	CG	ASP	438	14.996	69.498	33.543	1.00	41.58	A	C
ATOM	3334	OD1	ASP	438	15.820	69.415	34.480	1.00	43.35	A	O
ATOM	3335	OD2	ASP	438	13.796	69.785	33.725	1.00	43.71	A	O
ATOM	3336	C	ASP	438	17.904	69.470	32.700	1.00	35.28	A	C
ATOM	3337	O	ASP	438	18.019	68.274	32.993	1.00	33.70	A	O
ATOM	3338	N	TYR	439	18.723	70.412	33.158	1.00	34.27	A	N
ATOM	3339	CA	TYR	439	19.862	70.105	34.013	1.00	33.69	A	C
ATOM	3340	CB	TYR	439	20.740	71.343	34.175	1.00	32.29	A	C
ATOM	3341	CG	TYR	439	21.262	71.886	32.867	1.00	30.75	A	C
ATOM	3342	CD1	TYR	439	21.565	71.028	31.810	1.00	30.00	A	C
ATOM	3343	CE1	TYR	439	22.071	71.516	30.611	1.00	28.65	A	C
ATOM	3344	CD2	TYR	439	21.480	73.253	32.691	1.00	28.95	A	C
ATOM	3345	CE2	TYR	439	21.987	73.749	31.496	1.00	27.97	A	C
ATOM	3346	CZ	TYR	439	22.281	72.875	30.462	1.00	27.72	A	C
ATOM	3347	OH	TYR	439	22.803	73.350	29.284	1.00	28.72	A	O
ATOM	3348	C	TYR	439	19.543	69.538	35.390	1.00	33.65	A	C
ATOM	3349	O	TYR	439	20.435	69.045	36.076	1.00	33.49	A	O
ATOM	3350	N	THR	440	18.285	69.612	35.806	1.00	34.13	A	N
ATOM	3351	CA	THR	440	17.917	69.076	37.115	1.00	34.14	A	C
ATOM	3352	CB	THR	440	16.561	69.624	37.609	1.00	33.49	A	C
ATOM	3353	OG1	THR	440	15.507	69.114	36.780	1.00	32.29	A	O
ATOM	3354	CG2	THR	440	16.559	71.144	37.571	1.00	30.29	A	C
ATOM	3355	C	THR	440	17.794	67.572	36.953	1.00	33.89	A	C
ATOM	3356	O	THR	440	17.684	66.829	37.929	1.00	35.16	A	O
ATOM	3357	N	LYS	441	17.808	67.141	35.697	1.00	32.21	A	N
ATOM	3358	CA	LYS	441	17.703	65.735	35.362	1.00	30.32	A	C
ATOM	3359	CB	LYS	441	16.871	65.573	34.088	1.00	33.16	A	C
ATOM	3360	CG	LYS	441	15.369	65.490	34.331	1.00	36.13	A	C
ATOM	3361	CD	LYS	441	14.848	66.671	35.122	1.00	39.11	A	C
ATOM	3362	CE	LYS	441	13.447	66.392	35.649	1.00	41.94	A	C
ATOM	3363	NZ	LYS	441	12.953	67.501	36.517	1.00	44.46	A	N
ATOM	3364	C	LYS	441	19.089	65.119	35.179	1.00	28.77	A	C
ATOM	3365	O	LYS	441	19.668	65.159	34.088	1.00	28.32	A	O
ATOM	3366	N	VAL	442	19.618	64.564	36.263	1.00	25.14	A	N
ATOM	3367	CA	VAL	442	20.922	63.929	36.243	1.00	24.37	A	C
ATOM	3368	CB	VAL	442	21.960	64.717	37.091	1.00	24.82	A	C
ATOM	3369	CG1	VAL	442	23.266	63.936	37.178	1.00	22.99	A	C
ATOM	3370	CG2	VAL	442	22.216	66.084	36.469	1.00	23.65	A	C
ATOM	3371	C	VAL	442	20.786	62.525	36.807	1.00	24.10	A	C
ATOM	3372	O	VAL	442	20.327	62.341	37.931	1.00	22.60	A	O
ATOM	3373	N	THR	443	21.189	61.539	36.014	1.00	23.16	A	N
ATOM	3374	CA	THR	443	21.109	60.149	36.419	1.00	22.78	A	C
ATOM	3375	CB	THR	443	20.352	59.306	35.375	1.00	23.02	A	C
ATOM	3376	OG1	THR	443	19.017	59.802	35.222	1.00	27.68	A	O
ATOM	3377	CG2	THR	443	20.301	57.862	35.800	1.00	22.12	A	C
ATOM	3378	C	THR	443	22.493	59.548	36.551	1.00	23.54	A	C
ATOM	3379	O	THR	443	23.367	59.792	35.721	1.00	23.36	A	O
ATOM	3380	N	CYS	444	22.701	58.761	37.596	1.00	23.18	A	N

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(Continued)

## FIG. 4 - 70

ATOM	3381	CA	CYS	444	23.981	58.104	37.747	1.00	24.13	A	C
ATOM	3382	C	CYS	444	23.758	56.712	37.157	1.00	22.91	A	C
ATOM	3383	O	CYS	444	22.855	55.990	37.573	1.00	21.72	A	O
ATOM	3384	CB	CYS	444	24.396	58.018	39.219	1.00	25.50	A	C
ATOM	3385	SG	CYS	444	26.053	57.282	39.443	1.00	30.81	A	S
ATOM	3386	N	LEU	445	24.573	56.348	36.175	1.00	22.64	A	N
ATOM	3387	CA	LEU	445	24.446	55.053	35.513	1.00	22.51	A	C
ATOM	3388	CB	LEU	445	24.799	55.211	34.035	1.00	19.29	A	C
ATOM	3389	CG	LEU	445	24.049	56.349	33.341	1.00	19.36	A	C
ATOM	3390	CD1	LEU	445	24.588	56.552	31.934	1.00	16.01	A	C
ATOM	3391	CD2	LEU	445	22.559	56.034	33.319	1.00	15.72	A	C
ATOM	3392	C	LEU	445	25.308	53.940	36.118	1.00	23.32	A	C
ATOM	3393	O	LEU	445	25.203	52.783	35.718	1.00	24.58	A	O
ATOM	3394	N	SER	446	26.148	54.274	37.087	1.00	23.95	A	N
ATOM	3395	CA	SER	446	27.028	53.269	37.660	1.00	23.89	A	C
ATOM	3396	CB	SER	446	28.469	53.555	37.222	1.00	21.87	A	C
ATOM	3397	OG	SER	446	28.882	54.847	37.648	1.00	20.09	A	O
ATOM	3398	C	SER	446	26.969	53.145	39.175	1.00	23.77	A	C
ATOM	3399	O	SER	446	27.361	52.119	39.720	1.00	24.69	A	O
ATOM	3400	N	CYS	447	26.480	54.184	39.845	1.00	24.32	A	N
ATOM	3401	CA	CYS	447	26.382	54.207	41.309	1.00	26.45	A	C
ATOM	3402	C	CYS	447	25.836	52.946	41.997	1.00	25.99	A	C
ATOM	3403	O	CYS	447	26.441	52.425	42.937	1.00	24.44	A	O
ATOM	3404	CB	CYS	447	25.518	55.396	41.763	1.00	27.33	A	C
ATOM	3405	SG	CYS	447	26.225	57.049	41.461	1.00	34.75	A	S
ATOM	3406	N	GLU	448	24.696	52.456	41.528	1.00	25.90	A	N
ATOM	3407	CA	GLU	448	24.056	51.317	42.167	1.00	24.38	A	C
ATOM	3408	CB	GLU	448	22.581	51.637	42.334	1.00	23.47	A	C
ATOM	3409	CG	GLU	448	22.332	53.075	42.721	1.00	24.60	A	C
ATOM	3410	CD	GLU	448	22.848	53.416	44.108	1.00	27.44	A	C
ATOM	3411	OE1	GLU	448	22.617	54.562	44.559	1.00	29.17	A	O
ATOM	3412	OE2	GLU	448	23.478	52.548	44.751	1.00	28.81	A	O
ATOM	3413	C	GLU	448	24.201	49.941	41.537	1.00	23.54	A	C
ATOM	3414	O	GLU	448	23.722	48.970	42.104	1.00	22.25	A	O
ATOM	3415	N	LEU	449	24.844	49.844	40.377	1.00	23.78	A	N
ATOM	3416	CA	LEU	449	25.024	48.547	39.717	1.00	23.34	A	C
ATOM	3417	CB	LEU	449	25.988	48.678	38.548	1.00	20.76	A	C
ATOM	3418	CG	LEU	449	25.680	49.712	37.472	1.00	21.20	A	C
ATOM	3419	CD1	LEU	449	26.872	49.807	36.543	1.00	20.05	A	C
ATOM	3420	CD2	LEU	449	24.424	49.335	36.711	1.00	17.29	A	C
ATOM	3421	C	LEU	449	25.551	47.456	40.654	1.00	24.61	A	C
ATOM	3422	O	LEU	449	25.157	46.298	40.549	1.00	26.01	A	O
ATOM	3423	N	ASN	450	26.445	47.830	41.562	1.00	25.89	A	N
ATOM	3424	CA	ASN	450	27.040	46.889	42.512	1.00	27.02	A	C
ATOM	3425	CB	ASN	450	27.939	45.913	41.754	1.00	27.92	A	C
ATOM	3426	CG	ASN	450	28.296	44.695	42.572	1.00	31.61	A	C
ATOM	3427	OD1	ASN	450	28.521	44.786	43.783	1.00	34.65	A	O
ATOM	3428	ND2	ASN	450	28.363	43.541	41.912	1.00	31.27	A	N
ATOM	3429	C	ASN	450	27.877	47.731	43.488	1.00	26.54	A	C

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(Continued)

ATOM	3430	O	ASN	450	29.099	47.637	43.523	1.00	26.25	A	O
ATOM	3431	N	PRO	451	27.210	48.558	44.303	1.00	27.04	A	N
ATOM	3432	CD	PRO	451	25.762	48.411	44.535	1.00	27.72	A	C
ATOM	3433	CA	PRO	451	27.796	49.465	45.296	1.00	27.49	A	C
ATOM	3434	CB	PRO	451	26.579	49.924	46.103	1.00	27.21	A	C
ATOM	3435	CG	PRO	451	25.638	48.765	45.989	1.00	25.73	A	C
ATOM	3436	C	PRO	451	28.938	48.983	46.187	1.00	28.75	A	C
ATOM	3437	O	PRO	451	29.877	49.737	46.433	1.00	30.69	A	O
ATOM	3438	N	GLU	452	28.873	47.746	46.666	1.00	29.54	A	N
ATOM	3439	CA	GLU	452	29.918	47.228	47.545	1.00	30.30	A	C
ATOM	3440	CB	GLU	452	29.453	45.937	48.232	1.00	33.99	A	C
ATOM	3441	CG	GLU	452	28.085	46.024	48.890	1.00	39.92	A	C
ATOM	3442	CD	GLU	452	27.817	44.848	49.813	1.00	45.87	A	C
ATOM	3443	OE1	GLU	452	28.084	43.693	49.402	1.00	47.97	A	O
ATOM	3444	OE2	GLU	452	27.336	45.076	50.948	1.00	47.68	A	O
ATOM	3445	C	GLU	452	31.221	46.946	46.816	1.00	29.63	A	C
ATOM	3446	O	GLU	452	32.308	47.199	47.344	1.00	30.27	A	O
ATOM	3447	N	ARG	453	31.099	46.425	45.600	1.00	27.01	A	N
ATOM	3448	CA	ARG	453	32.244	46.057	44.783	1.00	24.90	A	C
ATOM	3449	CB	ARG	453	31.950	44.728	44.085	1.00	23.08	A	C
ATOM	3450	CG	ARG	453	32.952	44.337	43.018	1.00	22.92	A	C
ATOM	3451	CD	ARG	453	32.602	42.995	42.381	1.00	20.49	A	C
ATOM	3452	NE	ARG	453	33.504	42.688	41.278	1.00	18.31	A	N
ATOM	3453	CZ	ARG	453	33.439	41.595	40.531	1.00	18.93	A	C
ATOM	3454	NH1	ARG	453	32.510	40.679	40.763	1.00	19.77	A	N
ATOM	3455	NH2	ARG	453	34.302	41.425	39.539	1.00	18.87	A	N
ATOM	3456	C	ARG	453	32.695	47.071	43.738	1.00	25.72	A	C
ATOM	3457	O	ARG	453	33.809	46.962	43.222	1.00	24.32	A	O
ATOM	3458	N	CYS	454	31.857	48.054	43.420	1.00	25.94	A	N
ATOM	3459	CA	CYS	454	32.233	49.012	42.385	1.00	25.49	A	C
ATOM	3460	C	CYS	454	32.038	50.473	42.699	1.00	24.24	A	C
ATOM	3461	O	CYS	454	30.922	50.970	42.688	1.00	26.79	A	O
ATOM	3462	CB	CYS	454	31.503	48.664	41.096	1.00	26.13	A	C
ATOM	3463	SG	CYS	454	32.156	47.128	40.401	1.00	30.12	A	S
ATOM	3464	N	GLN	455	33.143	51.165	42.942	1.00	22.97	A	N
ATOM	3465	CA	GLN	455	33.105	52.576	43.276	1.00	23.69	A	C
ATOM	3466	CB	GLN	455	33.536	52.761	44.736	1.00	23.41	A	C
ATOM	3467	CG	GLN	455	32.564	52.187	45.761	1.00	24.96	A	C
ATOM	3468	CD	GLN	455	33.177	52.065	47.150	1.00	29.34	A	C
ATOM	3469	OE1	GLN	455	33.981	52.907	47.574	1.00	30.98	A	O
ATOM	3470	NE2	GLN	455	32.790	51.022	47.872	1.00	28.59	A	N
ATOM	3471	C	GLN	455	33.992	53.425	42.360	1.00	24.57	A	C
ATOM	3472	O	GLN	455	33.837	54.645	42.294	1.00	27.40	A	O
ATOM	3473	N	TYR	456	34.919	52.787	41.654	1.00	22.57	A	N
ATOM	3474	CA	TYR	456	35.821	53.510	40.763	1.00	21.75	A	C
ATOM	3475	CB	TYR	456	37.270	53.187	41.124	1.00	20.47	A	C
ATOM	3476	CG	TYR	456	38.267	54.282	40.817	1.00	21.27	A	C
ATOM	3477	CD1	TYR	456	38.659	55.193	41.808	1.00	20.27	A	C
ATOM	3478	CE1	TYR	456	39.618	56.165	41.548	1.00	18.67	A	C

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(Continued)

## FIG. 4 - 72

ATOM	3479	CD2	TYR	456	38.858	54.385	39.552	1.00	19.29	A	C
ATOM	3480	CE2	TYR	456	39.812	55.353	39.284	1.00	16.18	A	C
ATOM	3481	CZ	TYR	456	40.190	56.236	40.283	1.00	18.92	A	C
ATOM	3482	OH	TYR	456	41.151	57.183	40.023	1.00	19.64	A	O
ATOM	3483	C	TYR	456	35.536	53.061	39.335	1.00	21.96	A	C
ATOM	3484	O	TYR	456	35.944	51.972	38.931	1.00	22.39	A	O
ATOM	3485	N	TYR	457	34.846	53.899	38.567	1.00	22.09	A	N
ATOM	3486	CA	TYR	457	34.499	53.540	37.196	1.00	20.82	A	C
ATOM	3487	CB	TYR	457	33.001	53.717	36.956	1.00	17.91	A	C
ATOM	3488	CG	TYR	457	32.147	52.613	37.512	1.00	15.58	A	C
ATOM	3489	CD1	TYR	457	31.644	52.674	38.811	1.00	13.21	A	C
ATOM	3490	CE1	TYR	457	30.830	51.668	39.311	1.00	12.43	A	C
ATOM	3491	CD2	TYR	457	31.819	51.512	36.727	1.00	16.86	A	C
ATOM	3492	CE2	TYR	457	31.008	50.497	37.219	1.00	15.29	A	C
ATOM	3493	CZ	TYR	457	30.518	50.582	38.507	1.00	14.49	A	C
ATOM	3494	OH	TYR	457	29.728	49.568	38.985	1.00	15.62	A	O
ATOM	3495	C	TYR	457	35.232	54.240	36.066	1.00	21.27	A	C
ATOM	3496	O	TYR	457	35.842	55.293	36.227	1.00	23.18	A	O
ATOM	3497	N	SER	458	35.132	53.622	34.901	1.00	21.68	A	N
ATOM	3498	CA	SER	458	35.739	54.108	33.683	1.00	21.74	A	C
ATOM	3499	CB	SER	458	37.083	53.429	33.474	1.00	23.93	A	C
ATOM	3500	OG	SER	458	37.510	53.569	32.141	1.00	29.63	A	O
ATOM	3501	C	SER	458	34.751	53.664	32.621	1.00	21.73	A	C
ATOM	3502	O	SER	458	34.072	52.652	32.804	1.00	20.08	A	O
ATOM	3503	N	VAL	459	34.665	54.405	31.520	1.00	20.58	A	N
ATOM	3504	CA	VAL	459	33.722	54.061	30.468	1.00	19.99	A	C
ATOM	3505	CB	VAL	459	32.457	54.949	30.568	1.00	19.45	A	C
ATOM	3506	CG1	VAL	459	32.816	56.392	30.308	1.00	19.10	A	C
ATOM	3507	CG2	VAL	459	31.397	54.475	29.595	1.00	20.30	A	C
ATOM	3508	C	VAL	459	34.309	54.161	29.059	1.00	19.99	A	C
ATOM	3509	O	VAL	459	35.314	54.835	28.831	1.00	21.13	A	O
ATOM	3510	N	SER	460	33.667	53.472	28.122	1.00	18.73	A	N
ATOM	3511	CA	SER	460	34.083	53.456	26.728	1.00	16.25	A	C
ATOM	3512	CB	SER	460	34.970	52.230	26.476	1.00	16.33	A	C
ATOM	3513	OG	SER	460	35.476	52.194	25.151	1.00	15.85	A	O
ATOM	3514	C	SER	460	32.809	53.377	25.883	1.00	15.70	A	C
ATOM	3515	O	SER	460	32.156	52.342	25.841	1.00	14.81	A	O
ATOM	3516	N	PHE	461	32.450	54.475	25.226	1.00	16.00	A	N
ATOM	3517	CA	PHE	461	31.245	54.512	24.398	1.00	16.27	A	C
ATOM	3518	CB	PHE	461	30.636	55.921	24.367	1.00	15.50	A	C
ATOM	3519	CG	PHE	461	30.001	56.351	25.660	1.00	15.11	A	C
ATOM	3520	CD1	PHE	461	30.779	56.764	26.735	1.00	14.16	A	C
ATOM	3521	CD2	PHE	461	28.617	56.340	25.804	1.00	14.86	A	C
ATOM	3522	CE1	PHE	461	30.190	57.158	27.931	1.00	12.94	A	C
ATOM	3523	CE2	PHE	461	28.021	56.733	26.996	1.00	12.76	A	C
ATOM	3524	CZ	PHE	461	28.811	57.142	28.061	1.00	11.01	A	C
ATOM	3525	C	PHE	461	31.551	54.102	22.971	1.00	17.94	A	C
ATOM	3526	O	PHE	461	32.686	54.234	22.514	1.00	17.07	A	O
ATOM	3527	N	SER	462	30.532	53.612	22.269	1.00	19.22	A	N

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(Continued)

ATOM	3528	CA	SER	462	30.694	53.212	20.877	1.00	23.70	A	C
ATOM	3529	CB	SER	462	29.494	52.381	20.399	1.00	23.50	A	C
ATOM	3530	OG	SER	462	28.308	53.145	20.397	1.00	24.06	A	O
ATOM	3531	C	SER	462	30.804	54.496	20.058	1.00	24.95	A	C
ATOM	3532	O	SER	462	30.572	55.581	20.577	1.00	25.95	A	O
ATOM	3533	N	LYS	463	31.153	54.373	18.784	1.00	27.50	A	N
ATOM	3534	CA	LYS	463	31.323	55.536	17.920	1.00	31.80	A	C
ATOM	3535	CB	LYS	463	31.587	55.084	16.484	1.00	33.43	A	C
ATOM	3536	CG	LYS	463	33.047	55.199	16.075	1.00	35.54	A	C
ATOM	3537	CD	LYS	463	33.972	54.435	17.007	1.00	36.78	A	C
ATOM	3538	CE	LYS	463	35.433	54.724	16.673	1.00	39.20	A	C
ATOM	3539	NZ	LYS	463	36.384	54.098	17.641	1.00	40.26	A	N
ATOM	3540	C	LYS	463	30.226	56.602	17.934	1.00	33.39	A	C
ATOM	3541	O	LYS	463	30.484	57.745	17.561	1.00	36.36	A	O
ATOM	3542	N	GLU	464	29.015	56.254	18.354	1.00	33.23	A	N
ATOM	3543	CA	GLU	464	27.945	57.247	18.410	1.00	34.54	A	C
ATOM	3544	CB	GLU	464	26.960	57.058	17.256	1.00	39.82	A	C
ATOM	3545	CG	GLU	464	27.528	57.366	15.882	1.00	44.96	A	C
ATOM	3546	CD	GLU	464	26.578	56.961	14.772	1.00	48.72	A	C
ATOM	3547	OE1	GLU	464	25.439	57.480	14.752	1.00	50.39	A	O
ATOM	3548	OE2	GLU	464	26.967	56.120	13.926	1.00	50.59	A	O
ATOM	3549	C	GLU	464	27.186	57.202	19.729	1.00	32.77	A	C
ATOM	3550	O	GLU	464	26.047	57.659	19.814	1.00	32.03	A	O
ATOM	3551	N	ALA	465	27.823	56.636	20.748	1.00	31.17	A	N
ATOM	3552	CA	ALA	465	27.241	56.546	22.081	1.00	29.63	A	C
ATOM	3553	CB	ALA	465	26.889	57.935	22.577	1.00	28.36	A	C
ATOM	3554	C	ALA	465	26.015	55.645	22.164	1.00	29.47	A	C
ATOM	3555	O	ALA	465	25.176	55.824	23.042	1.00	28.66	A	O
ATOM	3556	N	LYS	466	25.905	54.678	21.259	1.00	28.89	A	N
ATOM	3557	CA	LYS	466	24.763	53.772	21.274	1.00	28.97	A	C
ATOM	3558	CB	LYS	466	24.585	53.122	19.899	1.00	30.98	A	C
ATOM	3559	CG	LYS	466	23.208	52.509	19.649	1.00	31.77	A	C
ATOM	3560	CD	LYS	466	23.045	52.179	18.171	1.00	34.52	A	C
ATOM	3561	CE	LYS	466	21.632	51.757	17.814	1.00	35.82	A	C
ATOM	3562	NZ	LYS	466	21.273	50.441	18.404	1.00	38.42	A	N
ATOM	3563	C	LYS	466	24.987	52.704	22.339	1.00	28.20	A	C
ATOM	3564	O	LYS	466	24.040	52.126	22.869	1.00	27.93	A	O
ATOM	3565	N	TYR	467	26.252	52.446	22.646	1.00	26.93	A	N
ATOM	3566	CA	TYR	467	26.599	51.458	23.654	1.00	26.21	A	C
ATOM	3567	CB	TYR	467	26.955	50.119	23.003	1.00	27.94	A	C
ATOM	3568	CG	TYR	467	25.823	49.502	22.207	1.00	30.39	A	C
ATOM	3569	CD1	TYR	467	25.550	49.917	20.903	1.00	29.93	A	C
ATOM	3570	CE1	TYR	467	24.494	49.373	20.184	1.00	31.13	A	C
ATOM	3571	CD2	TYR	467	25.009	48.522	22.768	1.00	29.73	A	C
ATOM	3572	CE2	TYR	467	23.953	47.975	22.060	1.00	30.29	A	C
ATOM	3573	CZ	TYR	467	23.698	48.405	20.770	1.00	30.97	A	C
ATOM	3574	OH	TYR	467	22.625	47.890	20.079	1.00	32.01	A	O
ATOM	3575	C	TYR	467	27.777	51.949	24.470	1.00	24.00	A	C
ATOM	3576	O	TYR	467	28.491	52.852	24.064	1.00	24.63	A	O

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(Continued)

## FIG. 4 - 74

ATOM	3577	N	TYR	468	27.969	51.370	25.641	1.00	23.06	A	N
ATOM	3578	CA	TYR	468	29.091	51.765	26.462	1.00	22.80	A	C
ATOM	3579	CB	TYR	468	28.801	53.043	27.249	1.00	23.88	A	C
ATOM	3580	CG	TYR	468	27.588	53.011	28.155	1.00	24.49	A	C
ATOM	3581	CD1	TYR	468	26.308	53.214	27.646	1.00	23.81	A	C
ATOM	3582	CE1	TYR	468	25.206	53.308	28.486	1.00	25.51	A	C
ATOM	3583	CD2	TYR	468	27.734	52.883	29.537	1.00	26.39	A	C
ATOM	3584	CE2	TYR	468	26.638	52.971	30.390	1.00	25.67	A	C
ATOM	3585	CZ	TYR	468	25.380	53.191	29.857	1.00	25.81	A	C
ATOM	3586	OH	TYR	468	24.304	53.334	30.695	1.00	25.95	A	O
ATOM	3587	C	TYR	468	29.501	50.675	27.411	1.00	21.32	A	C
ATOM	3588	O	TYR	468	28.672	50.059	28.070	1.00	22.73	A	O
ATOM	3589	N	GLN	469	30.800	50.431	27.449	1.00	20.26	A	N
ATOM	3590	CA	GLN	469	31.368	49.429	28.315	1.00	19.27	A	C
ATOM	3591	CB	GLN	469	32.643	48.864	27.695	1.00	20.12	A	C
ATOM	3592	CG	GLN	469	33.460	47.993	28.632	1.00	21.72	A	C
ATOM	3593	CD	GLN	469	34.891	47.845	28.169	1.00	23.85	A	C
ATOM	3594	OE1	GLN	469	35.605	48.837	28.011	1.00	25.81	A	O
ATOM	3595	NE2	GLN	469	35.322	46.609	27.948	1.00	23.84	A	N
ATOM	3596	C	GLN	469	31.712	50.158	29.589	1.00	19.50	A	C
ATOM	3597	O	GLN	469	32.331	51.226	29.549	1.00	19.63	A	O
ATOM	3598	N	LEU	470	31.277	49.611	30.716	1.00	19.27	A	N
ATOM	3599	CA	LEU	470	31.602	50.203	32.002	1.00	20.27	A	C
ATOM	3600	CB	LEU	470	30.410	50.136	32.961	1.00	20.14	A	C
ATOM	3601	CG	LEU	470	29.442	51.323	32.929	1.00	21.50	A	C
ATOM	3602	CD1	LEU	470	28.373	51.132	33.996	1.00	19.33	A	C
ATOM	3603	CD2	LEU	470	30.200	52.620	33.184	1.00	19.44	A	C
ATOM	3604	C	LEU	470	32.768	49.380	32.531	1.00	20.91	A	C
ATOM	3605	O	LEU	470	32.785	48.152	32.409	1.00	19.97	A	O
ATOM	3606	N	ARG	471	33.753	50.050	33.102	1.00	22.57	A	N
ATOM	3607	CA	ARG	471	34.917	49.344	33.610	1.00	25.83	A	C
ATOM	3608	CB	ARG	471	36.137	49.690	32.748	1.00	29.78	A	C
ATOM	3609	CG	ARG	471	35.927	49.386	31.261	1.00	31.73	A	C
ATOM	3610	CD	ARG	471	37.091	49.871	30.426	1.00	35.14	A	C
ATOM	3611	NE	ARG	471	36.939	51.261	30.005	1.00	35.86	A	N
ATOM	3612	CZ	ARG	471	37.961	52.061	29.723	1.00	35.39	A	C
ATOM	3613	NH1	ARG	471	39.202	51.606	29.830	1.00	37.87	A	N
ATOM	3614	NH2	ARG	471	37.747	53.304	29.321	1.00	36.33	A	N
ATOM	3615	C	ARG	471	35.171	49.686	35.064	1.00	24.89	A	C
ATOM	3616	O	ARG	471	35.685	50.750	35.388	1.00	27.07	A	O
ATOM	3617	N	CYS	472	34.794	48.766	35.935	1.00	24.59	A	N
ATOM	3618	CA	CYS	472	34.948	48.925	37.373	1.00	25.55	A	C
ATOM	3619	C	CYS	472	36.328	48.418	37.806	1.00	23.33	A	C
ATOM	3620	O	CYS	472	36.738	47.319	37.433	1.00	22.34	A	O
ATOM	3621	CB	CYS	472	33.812	48.150	38.059	1.00	26.66	A	C
ATOM	3622	SG	CYS	472	34.037	47.670	39.797	1.00	33.06	A	S
ATOM	3623	N	SER	473	37.049	49.219	38.583	1.00	22.51	A	N
ATOM	3624	CA	SER	473	38.377	48.809	39.022	1.00	23.17	A	C
ATOM	3625	CB	SER	473	39.446	49.724	38.414	1.00	21.92	A	C

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## FIG. 4 - 75

(Continued)

ATOM	3626	OG	SER	473	39.500	50.976	39.071	1.00	23.39	A	O
ATOM	3627	C	SER	473	38.557	48.754	40.536	1.00	23.29	A	C
ATOM	3628	O	SER	473	39.685	48.758	41.028	1.00	24.44	A	O
ATOM	3629	N	GLY	474	37.457	48.697	41.279	1.00	23.29	A	N
ATOM	3630	CA	GLY	474	37.573	48.627	42.724	1.00	23.91	A	C
ATOM	3631	C	GLY	474	36.330	49.075	43.459	1.00	24.41	A	C
ATOM	3632	O	GLY	474	35.434	49.658	42.849	1.00	25.28	A	O
ATOM	3633	N	PRO	475	36.257	48.850	44.780	1.00	24.58	A	N
ATOM	3634	CD	PRO	475	35.174	49.389	45.623	1.00	25.74	A	C
ATOM	3635	CA	PRO	475	37.280	48.206	45.609	1.00	24.00	A	C
ATOM	3636	CB	PRO	475	36.887	48.620	47.022	1.00	22.53	A	C
ATOM	3637	CG	PRO	475	35.419	48.692	46.945	1.00	25.59	A	C
ATOM	3638	C	PRO	475	37.397	46.692	45.462	1.00	24.86	A	C
ATOM	3639	O	PRO	475	38.294	46.081	46.044	1.00	26.60	A	O
ATOM	3640	N	GLY	476	36.502	46.085	44.691	1.00	24.35	A	N
ATOM	3641	CA	GLY	476	36.564	44.646	44.498	1.00	23.50	A	C
ATOM	3642	C	GLY	476	37.324	44.316	43.227	1.00	24.87	A	C
ATOM	3643	O	GLY	476	37.925	45.198	42.613	1.00	24.65	A	O
ATOM	3644	N	LEU	477	37.308	43.054	42.818	1.00	24.78	A	N
ATOM	3645	CA	LEU	477	38.003	42.681	41.601	1.00	25.85	A	C
ATOM	3646	CB	LEU	477	37.927	41.171	41.383	1.00	26.86	A	C
ATOM	3647	CG	LEU	477	38.661	40.296	42.404	1.00	27.45	A	C
ATOM	3648	CD1	LEU	477	38.626	38.851	41.943	1.00	27.65	A	C
ATOM	3649	CD2	LEU	477	40.102	40.759	42.556	1.00	27.87	A	C
ATOM	3650	C	LEU	477	37.369	43.417	40.424	1.00	27.45	A	C
ATOM	3651	O	LEU	477	36.160	43.663	40.405	1.00	27.68	A	O
ATOM	3652	N	PRO	478	38.183	43.792	39.428	1.00	27.18	A	N
ATOM	3653	CD	PRO	478	39.645	43.637	39.362	1.00	27.65	A	C
ATOM	3654	CA	PRO	478	37.684	44.505	38.253	1.00	25.83	A	C
ATOM	3655	CB	PRO	478	38.908	44.569	37.351	1.00	27.68	A	C
ATOM	3656	CG	PRO	478	40.023	44.676	38.335	1.00	27.43	A	C
ATOM	3657	C	PRO	478	36.509	43.806	37.591	1.00	24.68	A	C
ATOM	3658	O	PRO	478	36.464	42.583	37.506	1.00	23.74	A	O
ATOM	3659	N	LEU	479	35.561	44.600	37.116	1.00	24.02	A	N
ATOM	3660	CA	LEU	479	34.376	44.068	36.465	1.00	23.10	A	C
ATOM	3661	CB	LEU	479	33.186	44.151	37.420	1.00	21.62	A	C
ATOM	3662	CG	LEU	479	31.845	43.702	36.854	1.00	21.11	A	C
ATOM	3663	CD1	LEU	479	31.915	42.245	36.430	1.00	21.98	A	C
ATOM	3664	CD2	LEU	479	30.778	43.901	37.912	1.00	24.17	A	C
ATOM	3665	C	LEU	479	34.077	44.857	35.199	1.00	22.18	A	C
ATOM	3666	O	LEU	479	33.942	46.073	35.244	1.00	22.27	A	O
ATOM	3667	N	TYR	480	33.978	44.160	34.073	1.00	22.51	A	N
ATOM	3668	CA	TYR	480	33.690	44.801	32.790	1.00	22.76	A	C
ATOM	3669	CB	TYR	480	34.709	44.353	31.749	1.00	22.59	A	C
ATOM	3670	CG	TYR	480	36.123	44.657	32.147	1.00	21.95	A	C
ATOM	3671	CD1	TYR	480	36.702	45.885	31.843	1.00	22.81	A	C
ATOM	3672	CE1	TYR	480	37.999	46.190	32.249	1.00	23.84	A	C
ATOM	3673	CD2	TYR	480	36.872	43.733	32.870	1.00	22.05	A	C
ATOM	3674	CE2	TYR	480	38.165	44.027	33.286	1.00	23.52	A	C

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(Continued)

## FIG. 4 - 76

ATOM	3675	CZ	TYR	480	38.722	45.257	32.971	1.00	24.29	A	C
ATOM	3676	OH	TYR	480	39.998	45.556	33.379	1.00	26.37	A	O
ATOM	3677	C	TYR	480	32.291	44.422	32.326	1.00	23.22	A	C
ATOM	3678	O	TYR	480	31.964	43.239	32.243	1.00	23.21	A	O
ATOM	3679	N	THR	481	31.472	45.425	32.017	1.00	23.50	A	N
ATOM	3680	CA	THR	481	30.101	45.181	31.577	1.00	22.82	A	C
ATOM	3681	CB	THR	481	29.097	45.513	32.702	1.00	22.81	A	C
ATOM	3682	OG1	THR	481	29.190	46.905	33.024	1.00	23.28	A	O
ATOM	3683	CG2	THR	481	29.398	44.699	33.951	1.00	21.29	A	C
ATOM	3684	C	THR	481	29.740	46.015	30.351	1.00	23.25	A	C
ATOM	3685	O	THR	481	30.298	47.091	30.136	1.00	24.47	A	O
ATOM	3686	N	LEU	482	28.809	45.512	29.547	1.00	23.21	A	N
ATOM	3687	CA	LEU	482	28.368	46.219	28.350	1.00	23.54	A	C
ATOM	3688	CB	LEU	482	28.310	45.268	27.155	1.00	22.93	A	C
ATOM	3689	CG	LEU	482	28.216	45.922	25.773	1.00	23.14	A	C
ATOM	3690	CD1	LEU	482	29.483	46.721	25.507	1.00	23.20	A	C
ATOM	3691	CD2	LEU	482	28.043	44.861	24.699	1.00	22.53	A	C
ATOM	3692	C	LEU	482	26.981	46.767	28.643	1.00	23.83	A	C
ATOM	3693	O	LEU	482	26.254	46.207	29.458	1.00	25.57	A	O
ATOM	3694	N	HIS	483	26.610	47.861	27.994	1.00	22.84	A	N
ATOM	3695	CA	HIS	483	25.301	48.459	28.231	1.00	22.49	A	C
ATOM	3696	CB	HIS	483	25.420	49.528	29.321	1.00	22.16	A	C
ATOM	3697	CG	HIS	483	26.003	49.025	30.604	1.00	24.44	A	C
ATOM	3698	CD2	HIS	483	27.289	48.904	31.012	1.00	25.98	A	C
ATOM	3699	ND1	HIS	483	25.228	48.567	31.648	1.00	25.15	A	N
ATOM	3700	CE1	HIS	483	26.011	48.189	32.644	1.00	23.97	A	C
ATOM	3701	NE2	HIS	483	27.266	48.382	32.283	1.00	22.74	A	N
ATOM	3702	C	HIS	483	24.764	49.097	26.950	1.00	22.46	A	C
ATOM	3703	O	HIS	483	25.507	49.281	25.987	1.00	24.72	A	O
ATOM	3704	N	SER	484	23.475	49.427	26.932	1.00	20.23	A	N
ATOM	3705	CA	SER	484	22.890	50.078	25.768	1.00	19.27	A	C
ATOM	3706	CB	SER	484	21.789	49.216	25.164	1.00	19.99	A	C
ATOM	3707	OG	SER	484	20.721	49.057	26.068	1.00	26.06	A	O
ATOM	3708	C	SER	484	22.335	51.427	26.213	1.00	19.12	A	C
ATOM	3709	O	SER	484	21.656	51.521	27.232	1.00	19.17	A	O
ATOM	3710	N	SER	485	22.628	52.470	25.445	1.00	19.29	A	N
ATOM	3711	CA	SER	485	22.198	53.823	25.783	1.00	20.52	A	C
ATOM	3712	CB	SER	485	23.025	54.841	25.000	1.00	20.72	A	C
ATOM	3713	OG	SER	485	24.386	54.769	25.379	1.00	23.68	A	O
ATOM	3714	C	SER	485	20.727	54.160	25.604	1.00	20.05	A	C
ATOM	3715	O	SER	485	20.208	55.040	26.287	1.00	18.92	A	O
ATOM	3716	N	VAL	486	20.055	53.477	24.688	1.00	20.23	A	N
ATOM	3717	CA	VAL	486	18.653	53.764	24.444	1.00	19.23	A	C
ATOM	3718	CB	VAL	486	18.058	52.816	23.380	1.00	19.24	A	C
ATOM	3719	CG1	VAL	486	18.099	51.383	23.869	1.00	19.40	A	C
ATOM	3720	CG2	VAL	486	16.635	53.223	23.070	1.00	20.10	A	C
ATOM	3721	C	VAL	486	17.817	53.655	25.705	1.00	19.72	A	C
ATOM	3722	O	VAL	486	16.869	54.415	25.887	1.00	20.98	A	O
ATOM	3723	N	ASN	487	18.190	52.727	26.581	1.00	20.80	A	N

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## FIG. 4 - 77

(Continued)

ATOM	3724	CA	ASN	487	17.458	52.464	27.824	1.00	20.70	A	C
ATOM	3725	CB	ASN	487	16.587	51.229	27.620	1.00	18.89	A	C
ATOM	3726	CG	ASN	487	17.403	50.007	27.171	1.00	22.56	A	C
ATOM	3727	OD1	ASN	487	16.853	48.948	26.864	1.00	24.29	A	O
ATOM	3728	ND2	ASN	487	18.722	50.158	27.132	1.00	20.73	A	N
ATOM	3729	C	ASN	487	18.354	52.220	29.047	1.00	22.59	A	C
ATOM	3730	O	ASN	487	17.865	51.758	30.079	1.00	22.43	A	O
ATOM	3731	N	ASP	488	19.650	52.514	28.929	1.00	23.24	A	N
ATOM	3732	CA	ASP	488	20.606	52.290	30.015	1.00	23.32	A	C
ATOM	3733	CB	ASP	488	20.415	53.304	31.148	1.00	24.08	A	C
ATOM	3734	CG	ASP	488	20.780	54.718	30.750	1.00	24.71	A	C
ATOM	3735	OD1	ASP	488	21.933	54.956	30.345	1.00	25.68	A	O
ATOM	3736	OD2	ASP	488	19.907	55.601	30.862	1.00	26.77	A	O
ATOM	3737	C	ASP	488	20.488	50.883	30.608	1.00	24.38	A	C
ATOM	3738	O	ASP	488	20.709	50.689	31.803	1.00	24.38	A	O
ATOM	3739	N	LYS	489	20.127	49.902	29.791	1.00	24.63	A	N
ATOM	3740	CA	LYS	489	20.009	48.541	30.300	1.00	25.48	A	C
ATOM	3741	CB	LYS	489	18.837	47.817	29.630	1.00	25.85	A	C
ATOM	3742	CG	LYS	489	17.651	47.594	30.579	1.00	28.57	A	C
ATOM	3743	CD	LYS	489	17.247	48.906	31.251	1.00	30.67	A	C
ATOM	3744	CE	LYS	489	16.346	48.695	32.453	1.00	29.68	A	C
ATOM	3745	NZ	LYS	489	16.283	49.944	33.278	1.00	30.13	A	N
ATOM	3746	C	LYS	489	21.297	47.749	30.110	1.00	26.05	A	C
ATOM	3747	O	LYS	489	21.997	47.914	29.106	1.00	26.23	A	O
ATOM	3748	N	GLY	490	21.605	46.894	31.084	1.00	25.12	A	N
ATOM	3749	CA	GLY	490	22.812	46.094	31.019	1.00	23.91	A	C
ATOM	3750	C	GLY	490	22.694	44.966	30.017	1.00	25.29	A	C
ATOM	3751	O	GLY	490	21.855	44.082	30.172	1.00	27.16	A	O
ATOM	3752	N	LEU	491	23.531	44.991	28.986	1.00	24.58	A	N
ATOM	3753	CA	LEU	491	23.503	43.953	27.969	1.00	24.98	A	C
ATOM	3754	CB	LEU	491	24.298	44.385	26.737	1.00	25.21	A	C
ATOM	3755	CG	LEU	491	23.809	45.621	25.980	1.00	25.03	A	C
ATOM	3756	CD1	LEU	491	24.796	45.968	24.881	1.00	22.44	A	C
ATOM	3757	CD2	LEU	491	22.430	45.356	25.403	1.00	25.37	A	C
ATOM	3758	C	LEU	491	24.081	42.649	28.505	1.00	25.59	A	C
ATOM	3759	O	LEU	491	23.541	41.579	28.250	1.00	27.45	A	O
ATOM	3760	N	ARG	492	25.179	42.732	29.246	1.00	24.68	A	N
ATOM	3761	CA	ARG	492	25.798	41.529	29.780	1.00	24.07	A	C
ATOM	3762	CB	ARG	492	26.045	40.524	28.648	1.00	24.82	A	C
ATOM	3763	CG	ARG	492	27.159	40.919	27.666	1.00	26.62	A	C
ATOM	3764	CD	ARG	492	27.105	40.081	26.387	1.00	26.76	A	C
ATOM	3765	NE	ARG	492	25.884	40.357	25.641	1.00	29.45	A	N
ATOM	3766	CZ	ARG	492	25.708	41.414	24.855	1.00	30.52	A	C
ATOM	3767	NH1	ARG	492	26.684	42.297	24.692	1.00	31.57	A	N
ATOM	3768	NH2	ARG	492	24.540	41.610	24.261	1.00	29.62	A	N
ATOM	3769	C	ARG	492	27.117	41.831	30.473	1.00	23.83	A	C
ATOM	3770	O	ARG	492	27.602	42.958	30.438	1.00	22.78	A	O
ATOM	3771	N	VAL	493	27.680	40.807	31.109	1.00	24.93	A	N
ATOM	3772	CA	VAL	493	28.966	40.911	31.791	1.00	25.89	A	C

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(Continued)

## FIG. 4 - 78

ATOM	3773	CB	VAL	493	29.018	40.034	33.052	1.00	25.39	A	C
ATOM	3774	CG1	VAL	493	30.401	40.104	33.667	1.00	25.63	A	C
ATOM	3775	CG2	VAL	493	27.977	40.482	34.044	1.00	25.35	A	C
ATOM	3776	C	VAL	493	30.022	40.382	30.823	1.00	26.55	A	C
ATOM	3777	O	VAL	493	29.858	39.307	30.250	1.00	29.06	A	O
ATOM	3778	N	LEU	494	31.103	41.125	30.644	1.00	26.28	A	N
ATOM	3779	CA	LEU	494	32.154	40.705	29.731	1.00	25.35	A	C
ATOM	3780	CB	LEU	494	32.657	41.913	28.944	1.00	23.74	A	C
ATOM	3781	CG	LEU	494	31.611	42.554	28.031	1.00	22.82	A	C
ATOM	3782	CD1	LEU	494	32.017	43.989	27.697	1.00	22.34	A	C
ATOM	3783	CD2	LEU	494	31.453	41.706	26.769	1.00	19.11	A	C
ATOM	3784	C	LEU	494	33.315	40.034	30.453	1.00	26.29	A	C
ATOM	3785	O	LEU	494	34.001	39.182	29.885	1.00	29.20	A	O
ATOM	3786	N	GLU	495	33.536	40.420	31.703	1.00	24.94	A	N
ATOM	3787	CA	GLU	495	34.623	39.859	32.498	1.00	24.93	A	C
ATOM	3788	CB	GLU	495	35.969	40.445	32.060	1.00	24.61	A	C
ATOM	3789	CG	GLU	495	37.153	39.938	32.862	1.00	27.02	A	C
ATOM	3790	CD	GLU	495	37.332	38.435	32.733	1.00	29.02	A	C
ATOM	3791	OE1	GLU	495	37.263	37.724	33.760	1.00	29.22	A	O
ATOM	3792	OE2	GLU	495	37.539	37.962	31.596	1.00	30.56	A	O
ATOM	3793	C	GLU	495	34.357	40.210	33.951	1.00	25.32	A	C
ATOM	3794	O	GLU	495	34.146	41.380	34.285	1.00	24.97	A	O
ATOM	3795	N	ASP	496	34.358	39.197	34.809	1.00	25.38	A	N
ATOM	3796	CA	ASP	496	34.093	39.409	36.224	1.00	27.01	A	C
ATOM	3797	CB	ASP	496	32.761	38.757	36.602	1.00	27.17	A	C
ATOM	3798	CG	ASP	496	32.814	37.236	36.567	1.00	27.71	A	C
ATOM	3799	OD1	ASP	496	31.755	36.611	36.759	1.00	30.85	A	O
ATOM	3800	OD2	ASP	496	33.898	36.657	36.360	1.00	29.23	A	O
ATOM	3801	C	ASP	496	35.213	38.889	37.127	1.00	27.65	A	C
ATOM	3802	O	ASP	496	35.177	39.071	38.345	1.00	27.02	A	O
ATOM	3803	N	ASN	497	36.201	38.234	36.528	1.00	27.52	A	N
ATOM	3804	CA	ASN	497	37.329	37.717	37.287	1.00	29.40	A	C
ATOM	3805	CB	ASN	497	38.047	38.863	37.998	1.00	28.73	A	C
ATOM	3806	CG	ASN	497	38.973	39.622	37.080	1.00	29.26	A	C
ATOM	3807	OD1	ASN	497	39.988	39.093	36.630	1.00	27.48	A	O
ATOM	3808	ND2	ASN	497	38.628	40.870	36.792	1.00	31.42	A	N
ATOM	3809	C	ASN	497	36.946	36.652	38.301	1.00	30.77	A	C
ATOM	3810	O	ASN	497	37.407	36.669	39.444	1.00	31.70	A	O
ATOM	3811	N	SER	498	36.108	35.721	37.869	1.00	31.77	A	N
ATOM	3812	CA	SER	498	35.666	34.629	38.716	1.00	31.32	A	C
ATOM	3813	CB	SER	498	34.644	33.778	37.974	1.00	32.01	A	C
ATOM	3814	OG	SER	498	33.520	34.561	37.629	1.00	35.01	A	O
ATOM	3815	C	SER	498	36.854	33.772	39.093	1.00	30.55	A	C
ATOM	3816	O	SER	498	37.056	33.456	40.266	1.00	31.44	A	O
ATOM	3817	N	ALA	499	37.638	33.398	38.087	1.00	29.46	A	N
ATOM	3818	CA	ALA	499	38.814	32.566	38.304	1.00	29.07	A	C
ATOM	3819	CB	ALA	499	39.626	32.477	37.033	1.00	27.47	A	C
ATOM	3820	C	ALA	499	39.657	33.156	39.421	1.00	30.28	A	C
ATOM	3821	O	ALA	499	39.885	32.515	40.447	1.00	30.98	A	O

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## F I G. 4 - 7 9

(Continued)

ATOM	3822	N	LEU	500	40.098	34.393	39.223	1.00	30.98	A	N
ATOM	3823	CA	LEU	500	40.919	35.073	40.208	1.00	31.89	A	C
ATOM	3824	CB	LEU	500	41.218	36.502	39.755	1.00	31.32	A	C
ATOM	3825	CG	LEU	500	42.106	37.312	40.703	1.00	31.18	A	C
ATOM	3826	CD1	LEU	500	43.459	36.635	40.871	1.00	29.43	A	C
ATOM	3827	CD2	LEU	500	42.269	38.711	40.155	1.00	31.85	A	C
ATOM	3828	C	LEU	500	40.251	35.096	41.574	1.00	33.26	A	C
ATOM	3829	O	LEU	500	40.878	34.772	42.578	1.00	33.38	A	O
ATOM	3830	N	ASP	501	38.984	35.484	41.624	1.00	35.48	A	N
ATOM	3831	CA	ASP	501	38.294	35.522	42.905	1.00	38.46	A	C
ATOM	3832	CB	ASP	501	36.815	35.859	42.720	1.00	40.04	A	C
ATOM	3833	CG	ASP	501	36.068	35.942	44.043	1.00	42.67	A	C
ATOM	3834	OD1	ASP	501	36.349	36.870	44.831	1.00	44.51	A	O
ATOM	3835	OD2	ASP	501	35.202	35.076	44.300	1.00	44.58	A	O
ATOM	3836	C	ASP	501	38.432	34.149	43.557	1.00	39.76	A	C
ATOM	3837	O	ASP	501	38.622	34.039	44.765	1.00	39.03	A	O
ATOM	3838	N	LYS	502	38.352	33.103	42.740	1.00	41.28	A	N
ATOM	3839	CA	LYS	502	38.470	31.741	43.237	1.00	42.62	A	C
ATOM	3840	CB	LYS	502	38.206	30.746	42.100	1.00	44.22	A	C
ATOM	3841	CG	LYS	502	37.853	29.323	42.548	1.00	45.49	A	C
ATOM	3842	CD	LYS	502	39.071	28.557	43.050	1.00	47.22	A	C
ATOM	3843	CE	LYS	502	38.700	27.147	43.516	1.00	47.98	A	C
ATOM	3844	NZ	LYS	502	37.783	27.155	44.696	1.00	47.33	A	N
ATOM	3845	C	LYS	502	39.866	31.534	43.828	1.00	43.11	A	C
ATOM	3846	O	LYS	502	40.001	31.079	44.963	1.00	43.40	A	O
ATOM	3847	N	MET	503	40.900	31.881	43.064	1.00	42.72	A	N
ATOM	3848	CA	MET	503	42.280	31.735	43.528	1.00	43.17	A	C
ATOM	3849	CB	MET	503	43.256	32.193	42.444	1.00	45.35	A	C
ATOM	3850	CG	MET	503	43.267	31.332	41.200	1.00	48.35	A	C
ATOM	3851	SD	MET	503	44.396	32.004	39.952	1.00	54.36	A	S
ATOM	3852	CE	MET	503	45.957	31.226	40.438	1.00	52.89	A	C
ATOM	3853	C	MET	503	42.551	32.530	44.807	1.00	41.81	A	C
ATOM	3854	O	MET	503	43.059	31.990	45.790	1.00	40.44	A	O
ATOM	3855	N	LEU	504	42.215	33.815	44.779	1.00	41.12	A	N
ATOM	3856	CA	LEU	504	42.412	34.700	45.919	1.00	42.37	A	C
ATOM	3857	CB	LEU	504	41.914	36.103	45.566	1.00	41.90	A	C
ATOM	3858	CG	LEU	504	42.960	37.197	45.314	1.00	42.42	A	C
ATOM	3859	CD1	LEU	504	44.111	36.668	44.472	1.00	41.70	A	C
ATOM	3860	CD2	LEU	504	42.277	38.376	44.635	1.00	40.64	A	C
ATOM	3861	C	LEU	504	41.727	34.211	47.199	1.00	43.78	A	C
ATOM	3862	O	LEU	504	42.056	34.664	48.298	1.00	43.47	A	O
ATOM	3863	N	GLN	505	40.774	33.292	47.054	1.00	44.74	A	N
ATOM	3864	CA	GLN	505	40.053	32.737	48.198	1.00	45.12	A	C
ATOM	3865	CB	GLN	505	38.911	31.834	47.721	1.00	47.10	A	C
ATOM	3866	CG	GLN	505	37.767	32.574	47.059	1.00	50.85	A	C
ATOM	3867	CD	GLN	505	37.091	33.544	48.005	1.00	52.28	A	C
ATOM	3868	OE1	GLN	505	36.320	33.143	48.878	1.00	53.91	A	O
ATOM	3869	NE2	GLN	505	37.390	34.829	47.848	1.00	53.20	A	N
ATOM	3870	C	GLN	505	40.981	31.920	49.090	1.00	44.28	A	C

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(Continued)

## FIG. 4 - 80

ATOM	3871	O	GLN	505	40.806	31.863	50.309	1.00	44.07	A	O
ATOM	3872	N	ASN	506	41.970	31.288	48.473	1.00	43.04	A	N
ATOM	3873	CA	ASN	506	42.907	30.452	49.205	1.00	43.10	A	C
ATOM	3874	CB	ASN	506	43.301	29.254	48.344	1.00	47.04	A	C
ATOM	3875	CG	ASN	506	43.962	28.157	49.141	1.00	50.97	A	C
ATOM	3876	OD1	ASN	506	44.478	27.187	48.575	1.00	53.71	A	O
ATOM	3877	ND2	ASN	506	43.945	28.293	50.467	1.00	52.33	A	N
ATOM	3878	C	ASN	506	44.156	31.211	49.635	1.00	41.53	A	C
ATOM	3879	O	ASN	506	45.191	30.605	49.903	1.00	41.33	A	O
ATOM	3880	N	VAL	507	44.060	32.538	49.696	1.00	39.25	A	N
ATOM	3881	CA	VAL	507	45.186	33.367	50.110	1.00	35.74	A	C
ATOM	3882	CB	VAL	507	45.801	34.155	48.927	1.00	35.80	A	C
ATOM	3883	CG1	VAL	507	46.989	34.974	49.416	1.00	34.07	A	C
ATOM	3884	CG2	VAL	507	46.234	33.204	47.823	1.00	34.58	A	C
ATOM	3885	C	VAL	507	44.726	34.369	51.154	1.00	34.07	A	C
ATOM	3886	O	VAL	507	43.617	34.887	51.080	1.00	33.19	A	O
ATOM	3887	N	GLN	508	45.586	34.634	52.129	1.00	33.03	A	N
ATOM	3888	CA	GLN	508	45.272	35.578	53.191	1.00	31.62	A	C
ATOM	3889	CB	GLN	508	46.146	35.307	54.418	1.00	31.47	A	C
ATOM	3890	CG	GLN	508	46.034	33.894	54.970	1.00	31.59	A	C
ATOM	3891	CD	GLN	508	46.955	33.667	56.155	1.00	30.69	A	C
ATOM	3892	OE1	GLN	508	46.994	34.471	57.083	1.00	31.83	A	O
ATOM	3893	NE2	GLN	508	47.696	32.568	56.130	1.00	28.80	A	N
ATOM	3894	C	GLN	508	45.521	36.996	52.689	1.00	30.18	A	C
ATOM	3895	O	GLN	508	46.480	37.648	53.097	1.00	29.60	A	O
ATOM	3896	N	MET	509	44.652	37.463	51.801	1.00	28.77	A	N
ATOM	3897	CA	MET	509	44.775	38.797	51.236	1.00	28.64	A	C
ATOM	3898	CB	MET	509	43.744	38.993	50.124	1.00	30.06	A	C
ATOM	3899	CG	MET	509	44.004	38.143	48.896	1.00	31.71	A	C
ATOM	3900	SD	MET	509	45.605	38.540	48.171	1.00	34.08	A	S
ATOM	3901	CE	MET	509	45.130	39.727	46.922	1.00	30.89	A	C
ATOM	3902	C	MET	509	44.602	39.890	52.280	1.00	27.67	A	C
ATOM	3903	O	MET	509	43.875	39.724	53.255	1.00	28.41	A	O
ATOM	3904	N	PRO	510	45.279	41.032	52.085	1.00	26.51	A	N
ATOM	3905	CD	PRO	510	46.198	41.361	50.978	1.00	25.01	A	C
ATOM	3906	CA	PRO	510	45.180	42.150	53.023	1.00	24.17	A	C
ATOM	3907	CB	PRO	510	46.401	42.985	52.672	1.00	24.51	A	C
ATOM	3908	CG	PRO	510	46.442	42.847	51.185	1.00	23.21	A	C
ATOM	3909	C	PRO	510	43.881	42.896	52.741	1.00	23.17	A	C
ATOM	3910	O	PRO	510	43.209	42.632	51.751	1.00	24.30	A	O
ATOM	3911	N	SER	511	43.527	43.826	53.607	1.00	22.25	A	N
ATOM	3912	CA	SER	511	42.315	44.592	53.409	1.00	23.52	A	C
ATOM	3913	CB	SER	511	41.375	44.441	54.606	1.00	21.47	A	C
ATOM	3914	OG	SER	511	42.000	44.897	55.796	1.00	22.50	A	O
ATOM	3915	C	SER	511	42.734	46.043	53.258	1.00	25.81	A	C
ATOM	3916	O	SER	511	43.823	46.433	53.687	1.00	27.50	A	O
ATOM	3917	N	LYS	512	41.869	46.838	52.642	1.00	25.44	A	N
ATOM	3918	CA	LYS	512	42.148	48.242	52.437	1.00	24.17	A	C
ATOM	3919	CB	LYS	512	42.178	48.555	50.943	1.00	23.04	A	C

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(Continued)

## FIG. 4 - 81

ATOM	3920	CG	LYS	512	42.252	50.043	50.621	1.00	21.12	A	C
ATOM	3921	CD	LYS	512	42.368	50.249	49.125	1.00	21.07	A	C
ATOM	3922	CE	LYS	512	42.639	51.688	48.792	1.00	19.46	A	C
ATOM	3923	NZ	LYS	512	42.779	51.870	47.343	1.00	15.68	A	N
ATOM	3924	C	LYS	512	41.095	49.109	53.105	1.00	24.25	A	C
ATOM	3925	O	LYS	512	39.905	48.958	52.846	1.00	23.45	A	O
ATOM	3926	N	LYS	513	41.546	50.017	53.960	1.00	24.50	A	N
ATOM	3927	CA	LYS	513	40.661	50.941	54.647	1.00	25.28	A	C
ATOM	3928	CB	LYS	513	41.040	51.041	56.124	1.00	26.65	A	C
ATOM	3929	CG	LYS	513	40.202	52.025	56.914	1.00	27.55	A	C
ATOM	3930	CD	LYS	513	38.754	51.577	56.954	1.00	33.11	A	C
ATOM	3931	CE	LYS	513	37.901	52.476	57.844	1.00	35.12	A	C
ATOM	3932	NZ	LYS	513	36.503	51.943	57.960	1.00	38.12	A	N
ATOM	3933	C	LYS	513	40.806	52.312	53.999	1.00	26.42	A	C
ATOM	3934	O	LYS	513	41.918	52.829	53.877	1.00	28.66	A	O
ATOM	3935	N	LEU	514	39.688	52.891	53.575	1.00	25.40	A	N
ATOM	3936	CA	LEU	514	39.688	54.213	52.958	1.00	22.53	A	C
ATOM	3937	CB	LEU	514	39.147	54.119	51.536	1.00	20.88	A	C
ATOM	3938	CG	LEU	514	38.866	55.443	50.825	1.00	21.52	A	C
ATOM	3939	CD1	LEU	514	40.149	56.242	50.662	1.00	20.94	A	C
ATOM	3940	CD2	LEU	514	38.244	55.153	49.476	1.00	22.59	A	C
ATOM	3941	C	LEU	514	38.812	55.151	53.788	1.00	22.73	A	C
ATOM	3942	O	LEU	514	37.591	54.981	53.844	1.00	20.65	A	O
ATOM	3943	N	ASP	515	39.435	56.132	54.437	1.00	23.05	A	N
ATOM	3944	CA	ASP	515	38.693	57.076	55.268	1.00	25.43	A	C
ATOM	3945	CB	ASP	515	38.581	56.535	56.693	1.00	27.35	A	C
ATOM	3946	CG	ASP	515	37.419	57.142	57.458	1.00	30.82	A	C
ATOM	3947	OD1	ASP	515	37.278	56.851	58.668	1.00	32.73	A	O
ATOM	3948	OD2	ASP	515	36.639	57.905	56.851	1.00	32.89	A	O
ATOM	3949	C	ASP	515	39.346	58.462	55.287	1.00	26.80	A	C
ATOM	3950	O	ASP	515	40.054	58.835	54.357	1.00	27.23	A	O
ATOM	3951	N	PHE	516	39.107	59.230	56.345	1.00	27.53	A	N
ATOM	3952	CA	PHE	516	39.688	60.566	56.431	1.00	28.71	A	C
ATOM	3953	CB	PHE	516	38.780	61.590	55.729	1.00	28.60	A	C
ATOM	3954	CG	PHE	516	37.387	61.658	56.291	1.00	28.84	A	C
ATOM	3955	CD1	PHE	516	37.160	62.115	57.583	1.00	29.59	A	C
ATOM	3956	CD2	PHE	516	36.297	61.242	55.532	1.00	30.94	A	C
ATOM	3957	CE1	PHE	516	35.875	62.157	58.116	1.00	28.99	A	C
ATOM	3958	CE2	PHE	516	35.002	61.279	56.058	1.00	29.88	A	C
ATOM	3959	CZ	PHE	516	34.795	61.737	57.352	1.00	29.33	A	C
ATOM	3960	C	PHE	516	39.943	61.024	57.861	1.00	28.58	A	C
ATOM	3961	O	PHE	516	39.414	60.450	58.811	1.00	29.42	A	O
ATOM	3962	N	ILE	517	40.773	62.053	57.990	1.00	26.80	A	N
ATOM	3963	CA	ILE	517	41.094	62.651	59.272	1.00	28.68	A	C
ATOM	3964	CB	ILE	517	42.580	62.410	59.686	1.00	27.66	A	C
ATOM	3965	CG2	ILE	517	42.799	60.937	59.989	1.00	23.78	A	C
ATOM	3966	CG1	ILE	517	43.538	62.861	58.581	1.00	29.30	A	C
ATOM	3967	CD1	ILE	517	43.676	64.361	58.431	1.00	31.79	A	C
ATOM	3968	C	ILE	517	40.829	64.132	59.041	1.00	30.84	A	C

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(Continued)

## FIG. 4 - 82

ATOM	3969	O	ILE	517	40.813	64.577	57.898	1.00	31.70	A	O
ATOM	3970	N	ILE	518	40.616	64.899	60.102	1.00	32.28	A	N
ATOM	3971	CA	ILE	518	40.323	66.313	59.924	1.00	33.51	A	C
ATOM	3972	CB	ILE	518	38.977	66.683	60.595	1.00	33.41	A	C
ATOM	3973	CG2	ILE	518	38.603	68.125	60.283	1.00	33.29	A	C
ATOM	3974	CG1	ILE	518	37.871	65.765	60.072	1.00	33.38	A	C
ATOM	3975	CD1	ILE	518	36.535	65.972	60.749	1.00	33.46	A	C
ATOM	3976	C	ILE	518	41.415	67.222	60.455	1.00	35.00	A	C
ATOM	3977	O	ILE	518	41.883	67.069	61.580	1.00	35.82	A	O
ATOM	3978	N	LEU	519	41.824	68.169	59.622	1.00	36.74	A	N
ATOM	3979	CA	LEU	519	42.850	69.126	59.997	1.00	39.19	A	C
ATOM	3980	CB	LEU	519	44.169	68.828	59.276	1.00	38.52	A	C
ATOM	3981	CG	LEU	519	44.746	67.413	59.364	1.00	39.20	A	C
ATOM	3982	CD1	LEU	519	45.996	67.326	58.493	1.00	39.31	A	C
ATOM	3983	CD2	LEU	519	45.068	67.059	60.806	1.00	39.59	A	C
ATOM	3984	C	LEU	519	42.351	70.501	59.591	1.00	40.26	A	C
ATOM	3985	O	LEU	519	42.102	70.754	58.414	1.00	40.93	A	O
ATOM	3986	N	ASN	520	42.198	71.382	60.574	1.00	41.70	A	N
ATOM	3987	CA	ASN	520	41.736	72.735	60.321	1.00	42.46	A	C
ATOM	3988	CB	ASN	520	42.760	73.474	59.467	1.00	44.27	A	C
ATOM	3989	CG	ASN	520	44.078	73.635	60.177	1.00	46.04	A	C
ATOM	3990	OD1	ASN	520	44.540	72.723	60.859	1.00	47.21	A	O
ATOM	3991	ND2	ASN	520	44.697	74.796	60.020	1.00	50.39	A	N
ATOM	3992	C	ASN	520	40.384	72.728	59.638	1.00	42.18	A	C
ATOM	3993	O	ASN	520	40.183	73.388	58.620	1.00	42.15	A	O
ATOM	3994	N	GLU	521	39.461	71.963	60.210	1.00	41.73	A	N
ATOM	3995	CA	GLU	521	38.105	71.861	59.691	1.00	42.64	A	C
ATOM	3996	CB	GLU	521	37.445	73.245	59.660	1.00	44.72	A	C
ATOM	3997	CG	GLU	521	37.967	74.204	60.715	1.00	48.09	A	C
ATOM	3998	CD	GLU	521	38.057	73.564	62.081	1.00	50.91	A	C
ATOM	3999	OE1	GLU	521	36.994	73.245	62.661	1.00	52.95	A	O
ATOM	4000	OE2	GLU	521	39.194	73.374	62.568	1.00	51.94	A	O
ATOM	4001	C	GLU	521	38.041	71.248	58.296	1.00	40.90	A	C
ATOM	4002	O	GLU	521	36.967	71.171	57.701	1.00	40.88	A	O
ATOM	4003	N	THR	522	39.182	70.814	57.772	1.00	39.01	A	N
ATOM	4004	CA	THR	522	39.206	70.221	56.442	1.00	36.94	A	C
ATOM	4005	CB	THR	522	40.339	70.816	55.584	1.00	38.55	A	C
ATOM	4006	OG1	THR	522	40.127	72.223	55.431	1.00	40.51	A	O
ATOM	4007	CG2	THR	522	40.364	70.171	54.202	1.00	39.39	A	C
ATOM	4008	C	THR	522	39.357	68.706	56.482	1.00	34.94	A	C
ATOM	4009	O	THR	522	40.086	68.152	57.305	1.00	33.48	A	O
ATOM	4010	N	LYS	523	38.653	68.045	55.573	1.00	33.07	A	N
ATOM	4011	CA	LYS	523	38.685	66.597	55.479	1.00	30.63	A	C
ATOM	4012	CB	LYS	523	37.357	66.105	54.901	1.00	31.78	A	C
ATOM	4013	CG	LYS	523	36.882	64.770	55.440	1.00	34.92	A	C
ATOM	4014	CD	LYS	523	35.473	64.458	54.956	1.00	37.12	A	C
ATOM	4015	CE	LYS	523	34.473	65.488	55.455	1.00	40.20	A	C
ATOM	4016	NZ	LYS	523	33.111	65.296	54.873	1.00	43.74	A	N
ATOM	4017	C	LYS	523	39.845	66.191	54.576	1.00	28.84	A	C

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## F I G. 4 - 8 3

ATOM	4018	O	LYS	523	39.962	66.661	53.448	1.00	29.90	A	O
ATOM	4019	N	PHE	524	40.711	65.329	55.086	1.00	26.11	A	N
ATOM	4020	CA	PHE	524	41.857	64.858	54.334	1.00	23.17	A	C
ATOM	4021	CB	PHE	524	43.139	65.407	54.953	1.00	22.95	A	C
ATOM	4022	CG	PHE	524	43.394	66.854	54.636	1.00	21.35	A	C
ATOM	4023	CD1	PHE	524	43.773	67.242	53.346	1.00	21.14	A	C
ATOM	4024	CD2	PHE	524	43.265	67.830	55.620	1.00	18.86	A	C
ATOM	4025	CE1	PHE	524	44.026	68.587	53.040	1.00	19.22	A	C
ATOM	4026	CE2	PHE	524	43.512	69.171	55.329	1.00	19.37	A	C
ATOM	4027	CZ	PHE	524	43.895	69.552	54.034	1.00	19.34	A	C
ATOM	4028	C	PHE	524	41.872	63.337	54.328	1.00	23.15	A	C
ATOM	4029	O	PHE	524	42.084	62.703	55.356	1.00	22.01	A	O
ATOM	4030	N	TRP	525	41.640	62.758	53.156	1.00	24.00	A	N
ATOM	4031	CA	TRP	525	41.593	61.309	53.000	1.00	23.65	A	C
ATOM	4032	CB	TRP	525	40.875	60.958	51.696	1.00	23.74	A	C
ATOM	4033	CG	TRP	525	39.476	61.452	51.647	1.00	24.69	A	C
ATOM	4034	CD2	TRP	525	38.291	60.687	51.893	1.00	25.25	A	C
ATOM	4035	CE2	TRP	525	37.195	61.572	51.800	1.00	26.02	A	C
ATOM	4036	CE3	TRP	525	38.049	59.339	52.186	1.00	25.53	A	C
ATOM	4037	CD1	TRP	525	39.065	62.732	51.418	1.00	25.58	A	C
ATOM	4038	NE1	TRP	525	37.693	62.815	51.508	1.00	25.32	A	N
ATOM	4039	CZ2	TRP	525	35.874	61.151	51.990	1.00	25.72	A	C
ATOM	4040	CZ3	TRP	525	36.735	58.919	52.374	1.00	24.54	A	C
ATOM	4041	CH2	TRP	525	35.666	59.824	52.276	1.00	24.86	A	C
ATOM	4042	C	TRP	525	42.927	60.566	53.042	1.00	23.39	A	C
ATOM	4043	O	TRP	525	43.994	61.127	52.803	1.00	24.19	A	O
ATOM	4044	N	TYR	526	42.840	59.280	53.347	1.00	22.63	A	N
ATOM	4045	CA	TYR	526	44.002	58.412	53.410	1.00	22.38	A	C
ATOM	4046	CB	TYR	526	44.715	58.546	54.763	1.00	22.15	A	C
ATOM	4047	CG	TYR	526	43.946	57.946	55.929	1.00	24.08	A	C
ATOM	4048	CD1	TYR	526	43.968	56.574	56.178	1.00	23.01	A	C
ATOM	4049	CE1	TYR	526	43.215	56.017	57.204	1.00	25.01	A	C
ATOM	4050	CD2	TYR	526	43.150	58.748	56.747	1.00	24.62	A	C
ATOM	4051	CE2	TYR	526	42.395	58.205	57.772	1.00	24.74	A	C
ATOM	4052	CZ	TYR	526	42.426	56.840	57.997	1.00	25.67	A	C
ATOM	4053	OH	TYR	526	41.650	56.303	59.003	1.00	25.43	A	O
ATOM	4054	C	TYR	526	43.478	56.990	53.251	1.00	22.00	A	C
ATOM	4055	O	TYR	526	42.294	56.724	53.482	1.00	21.71	A	O
ATOM	4056	N	GLN	527	44.353	56.084	52.843	1.00	19.68	A	N
ATOM	4057	CA	GLN	527	43.964	54.697	52.707	1.00	20.14	A	C
ATOM	4058	CB	GLN	527	43.842	54.301	51.238	1.00	19.56	A	C
ATOM	4059	CG	GLN	527	45.123	54.422	50.465	1.00	23.06	A	C
ATOM	4060	CD	GLN	527	44.986	53.890	49.065	1.00	23.49	A	C
ATOM	4061	OE1	GLN	527	44.034	54.222	48.359	1.00	25.79	A	O
ATOM	4062	NE2	GLN	527	45.937	53.066	48.648	1.00	22.35	A	N
ATOM	4063	C	GLN	527	45.038	53.871	53.389	1.00	20.67	A	C
ATOM	4064	O	GLN	527	46.172	54.334	53.563	1.00	19.72	A	O
ATOM	4065	N	MET	528	44.674	52.659	53.792	1.00	21.11	A	N
ATOM	4066	CA	MET	528	45.610	51.771	54.460	1.00	22.32	A	C

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(Continued)

## FIG. 4 - 84

ATOM	4067	CB	MET	528	45.372	51.753	55.967	1.00	23.57	A	C
ATOM	4068	CG	MET	528	45.830	52.971	56.727	1.00	23.53	A	C
ATOM	4069	SD	MET	528	45.605	52.683	58.492	1.00	23.56	A	S
ATOM	4070	CE	MET	528	46.400	54.107	59.158	1.00	21.91	A	C
ATOM	4071	C	MET	528	45.482	50.347	53.974	1.00	23.25	A	C
ATOM	4072	O	MET	528	44.383	49.790	53.935	1.00	24.82	A	O
ATOM	4073	N	ILE	529	46.605	49.751	53.600	1.00	22.51	A	N
ATOM	4074	CA	ILE	529	46.587	48.363	53.183	1.00	21.97	A	C
ATOM	4075	CB	ILE	529	47.644	48.078	52.116	1.00	19.54	A	C
ATOM	4076	CG2	ILE	529	47.557	46.635	51.681	1.00	18.75	A	C
ATOM	4077	CG1	ILE	529	47.454	49.029	50.927	1.00	21.01	A	C
ATOM	4078	CD1	ILE	529	46.045	49.038	50.335	1.00	19.28	A	C
ATOM	4079	C	ILE	529	46.937	47.620	54.465	1.00	24.02	A	C
ATOM	4080	O	ILE	529	48.114	47.505	54.820	1.00	25.51	A	O
ATOM	4081	N	LEU	530	45.911	47.153	55.175	1.00	24.47	A	N
ATOM	4082	CA	LEU	530	46.114	46.443	56.438	1.00	24.76	A	C
ATOM	4083	CB	LEU	530	44.915	46.640	57.370	1.00	24.08	A	C
ATOM	4084	CG	LEU	530	44.451	48.052	57.726	1.00	24.92	A	C
ATOM	4085	CD1	LEU	530	43.365	47.928	58.763	1.00	26.76	A	C
ATOM	4086	CD2	LEU	530	45.589	48.896	58.272	1.00	25.50	A	C
ATOM	4087	C	LEU	530	46.337	44.953	56.241	1.00	24.39	A	C
ATOM	4088	O	LEU	530	45.686	44.319	55.411	1.00	24.58	A	O
ATOM	4089	N	PRO	531	47.272	44.374	57.003	1.00	24.58	A	N
ATOM	4090	CD	PRO	531	48.174	45.045	57.950	1.00	24.42	A	C
ATOM	4091	CA	PRO	531	47.578	42.943	56.913	1.00	26.79	A	C
ATOM	4092	CB	PRO	531	48.763	42.784	57.862	1.00	26.36	A	C
ATOM	4093	CG	PRO	531	48.580	43.913	58.838	1.00	26.79	A	C
ATOM	4094	C	PRO	531	46.388	42.078	57.312	1.00	28.05	A	C
ATOM	4095	O	PRO	531	45.443	42.562	57.931	1.00	31.01	A	O
ATOM	4096	N	PRO	532	46.417	40.782	56.964	1.00	28.42	A	N
ATOM	4097	CD	PRO	532	47.484	40.062	56.253	1.00	28.00	A	C
ATOM	4098	CA	PRO	532	45.316	39.874	57.306	1.00	28.68	A	C
ATOM	4099	CB	PRO	532	45.783	38.534	56.745	1.00	28.68	A	C
ATOM	4100	CG	PRO	532	46.726	38.912	55.659	1.00	28.50	A	C
ATOM	4101	C	PRO	532	45.113	39.799	58.814	1.00	29.80	A	C
ATOM	4102	O	PRO	532	46.051	40.006	59.579	1.00	31.52	A	O
ATOM	4103	N	HIS	533	43.894	39.501	59.242	1.00	31.29	A	N
ATOM	4104	CA	HIS	533	43.605	39.382	60.670	1.00	31.80	A	C
ATOM	4105	CB	HIS	533	44.278	38.127	61.225	1.00	29.82	A	C
ATOM	4106	CG	HIS	533	44.170	36.936	60.324	1.00	29.23	A	C
ATOM	4107	CD2	HIS	533	45.114	36.247	59.641	1.00	28.40	A	C
ATOM	4108	ND1	HIS	533	42.966	36.335	60.024	1.00	28.40	A	N
ATOM	4109	CE1	HIS	533	43.174	35.326	59.197	1.00	28.67	A	C
ATOM	4110	NE2	HIS	533	44.469	35.251	58.949	1.00	28.85	A	N
ATOM	4111	C	HIS	533	44.101	40.601	61.445	1.00	33.77	A	C
ATOM	4112	O	HIS	533	44.469	40.489	62.617	1.00	33.99	A	O
ATOM	4113	N	PHE	534	44.121	41.758	60.787	1.00	35.52	A	N
ATOM	4114	CA	PHE	534	44.578	42.987	61.427	1.00	37.29	A	C
ATOM	4115	CB	PHE	534	44.249	44.203	60.555	1.00	36.11	A	C

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## FIG. 4 - 85

(Continued)

ATOM	4116	CG	PHE	534	44.510	45.523	61.235	1.00	35.46	A	C
ATOM	4117	CD1	PHE	534	45.811	45.956	61.475	1.00	35.65	A	C
ATOM	4118	CD2	PHE	534	43.455	46.320	61.654	1.00	33.35	A	C
ATOM	4119	CE1	PHE	534	46.056	47.167	62.124	1.00	36.55	A	C
ATOM	4120	CE2	PHE	534	43.688	47.530	62.304	1.00	35.26	A	C
ATOM	4121	CZ	PHE	534	44.990	47.957	62.541	1.00	35.35	A	C
ATOM	4122	C	PHE	534	43.920	43.158	62.790	1.00	38.07	A	C
ATOM	4123	O	PHE	534	42.705	43.046	62.911	1.00	38.83	A	O
ATOM	4124	N	ASP	535	44.725	43.435	63.810	1.00	39.27	A	N
ATOM	4125	CA	ASP	535	44.206	43.621	65.160	1.00	40.72	A	C
ATOM	4126	CB	ASP	535	44.751	42.541	66.089	1.00	43.14	A	C
ATOM	4127	CG	ASP	535	44.102	42.571	67.460	1.00	46.19	A	C
ATOM	4128	OD1	ASP	535	43.704	43.668	67.912	1.00	46.58	A	O
ATOM	4129	OD2	ASP	535	43.999	41.499	68.092	1.00	48.00	A	O
ATOM	4130	C	ASP	535	44.614	44.985	65.699	1.00	40.91	A	C
ATOM	4131	O	ASP	535	45.799	45.270	65.837	1.00	40.57	A	O
ATOM	4132	N	LYS	536	43.635	45.822	66.022	1.00	41.40	A	N
ATOM	4133	CA	LYS	536	43.936	47.148	66.539	1.00	42.56	A	C
ATOM	4134	CB	LYS	536	42.675	48.018	66.572	1.00	44.69	A	C
ATOM	4135	CG	LYS	536	42.146	48.406	65.200	1.00	47.06	A	C
ATOM	4136	CD	LYS	536	41.156	49.566	65.289	1.00	49.52	A	C
ATOM	4137	CE	LYS	536	40.721	50.020	63.897	1.00	50.85	A	C
ATOM	4138	NZ	LYS	536	39.965	51.303	63.921	1.00	51.05	A	N
ATOM	4139	C	LYS	536	44.553	47.105	67.928	1.00	42.57	A	C
ATOM	4140	O	LYS	536	44.896	48.147	68.486	1.00	42.20	A	O
ATOM	4141	N	SER	537	44.697	45.907	68.486	1.00	42.80	A	N
ATOM	4142	CA	SER	537	45.277	45.762	69.820	1.00	43.70	A	C
ATOM	4143	CB	SER	537	44.744	44.499	70.513	1.00	44.09	A	C
ATOM	4144	OG	SER	537	45.222	43.319	69.888	1.00	43.50	A	O
ATOM	4145	C	SER	537	46.796	45.696	69.737	1.00	43.27	A	C
ATOM	4146	O	SER	537	47.498	46.061	70.682	1.00	44.98	A	O
ATOM	4147	N	LYS	538	47.295	45.230	68.598	1.00	41.93	A	N
ATOM	4148	CA	LYS	538	48.729	45.110	68.380	1.00	40.13	A	C
ATOM	4149	CB	LYS	538	49.024	43.917	67.470	1.00	41.29	A	C
ATOM	4150	CG	LYS	538	48.521	42.590	68.013	1.00	42.24	A	C
ATOM	4151	CD	LYS	538	48.834	41.446	67.073	1.00	41.97	A	C
ATOM	4152	CE	LYS	538	48.317	40.140	67.638	1.00	42.57	A	C
ATOM	4153	NZ	LYS	538	46.864	40.231	67.960	1.00	44.10	A	N
ATOM	4154	C	LYS	538	49.280	46.372	67.741	1.00	38.59	A	C
ATOM	4155	O	LYS	538	48.526	47.229	67.283	1.00	38.17	A	O
ATOM	4156	N	LYS	539	50.601	46.485	67.725	1.00	36.92	A	N
ATOM	4157	CA	LYS	539	51.263	47.629	67.116	1.00	36.43	A	C
ATOM	4158	CB	LYS	539	52.293	48.225	68.079	1.00	37.32	A	C
ATOM	4159	CG	LYS	539	51.693	48.838	69.341	1.00	37.42	A	C
ATOM	4160	CD	LYS	539	50.925	50.117	69.028	1.00	40.01	A	C
ATOM	4161	CE	LYS	539	50.209	50.674	70.258	1.00	41.64	A	C
ATOM	4162	NZ	LYS	539	51.121	51.014	71.389	1.00	43.98	A	N
ATOM	4163	C	LYS	539	51.943	47.110	65.849	1.00	35.38	A	C
ATOM	4164	O	LYS	539	52.699	46.137	65.893	1.00	35.49	A	O

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(Continued)

## FIG. 4 - 86

ATOM	4165	N	TYR	540	51.658	47.747	64.719	1.00	33.00	A	N
ATOM	4166	CA	TYR	540	52.229	47.316	63.452	1.00	30.12	A	C
ATOM	4167	CB	TYR	540	51.131	47.135	62.397	1.00	28.99	A	C
ATOM	4168	CG	TYR	540	50.204	45.968	62.630	1.00	29.13	A	C
ATOM	4169	CD1	TYR	540	49.109	46.078	63.488	1.00	28.32	A	C
ATOM	4170	CE1	TYR	540	48.254	45.000	63.699	1.00	27.13	A	C
ATOM	4171	CD2	TYR	540	50.421	44.748	61.990	1.00	27.62	A	C
ATOM	4172	CE2	TYR	540	49.576	43.669	62.196	1.00	26.32	A	C
ATOM	4173	CZ	TYR	540	48.495	43.800	63.051	1.00	27.64	A	C
ATOM	4174	OH	TYR	540	47.661	42.724	63.260	1.00	29.67	A	O
ATOM	4175	C	TYR	540	53.242	48.287	62.890	1.00	29.33	A	C
ATOM	4176	O	TYR	540	53.130	49.492	63.091	1.00	31.23	A	O
ATOM	4177	N	PRO	541	54.270	47.772	62.199	1.00	27.71	A	N
ATOM	4178	CD	PRO	541	54.717	46.383	62.020	1.00	25.95	A	C
ATOM	4179	CA	PRO	541	55.238	48.708	61.634	1.00	27.56	A	C
ATOM	4180	CB	PRO	541	56.361	47.794	61.148	1.00	26.81	A	C
ATOM	4181	CG	PRO	541	55.662	46.512	60.867	1.00	25.92	A	C
ATOM	4182	C	PRO	541	54.463	49.358	60.500	1.00	27.83	A	C
ATOM	4183	O	PRO	541	53.579	48.727	59.912	1.00	28.03	A	O
ATOM	4184	N	LEU	542	54.763	50.613	60.200	1.00	27.70	A	N
ATOM	4185	CA	LEU	542	54.032	51.307	59.154	1.00	26.55	A	C
ATOM	4186	CB	LEU	542	53.220	52.440	59.791	1.00	26.11	A	C
ATOM	4187	CG	LEU	542	52.252	53.292	58.959	1.00	28.68	A	C
ATOM	4188	CD1	LEU	542	51.422	54.170	59.898	1.00	29.38	A	C
ATOM	4189	CD2	LEU	542	53.017	54.165	57.979	1.00	29.52	A	C
ATOM	4190	C	LEU	542	54.924	51.855	58.042	1.00	26.16	A	C
ATOM	4191	O	LEU	542	55.943	52.492	58.303	1.00	28.00	A	O
ATOM	4192	N	LEU	543	54.536	51.589	56.801	1.00	23.70	A	N
ATOM	4193	CA	LEU	543	55.263	52.097	55.651	1.00	24.11	A	C
ATOM	4194	CB	LEU	543	55.595	50.978	54.660	1.00	24.05	A	C
ATOM	4195	CG	LEU	543	56.080	51.474	53.289	1.00	22.45	A	C
ATOM	4196	CD1	LEU	543	57.209	52.487	53.475	1.00	24.00	A	C
ATOM	4197	CD2	LEU	543	56.537	50.303	52.441	1.00	20.16	A	C
ATOM	4198	C	LEU	543	54.378	53.131	54.966	1.00	24.37	A	C
ATOM	4199	O	LEU	543	53.283	52.819	54.511	1.00	25.72	A	O
ATOM	4200	N	LEU	544	54.857	54.362	54.896	1.00	24.80	A	N
ATOM	4201	CA	LEU	544	54.098	55.436	54.278	1.00	23.74	A	C
ATOM	4202	CB	LEU	544	54.424	56.757	54.979	1.00	23.92	A	C
ATOM	4203	CG	LEU	544	53.640	58.003	54.581	1.00	22.62	A	C
ATOM	4204	CD1	LEU	544	52.157	57.743	54.729	1.00	24.91	A	C
ATOM	4205	CD2	LEU	544	54.069	59.166	55.460	1.00	24.25	A	C
ATOM	4206	C	LEU	544	54.403	55.543	52.785	1.00	23.24	A	C
ATOM	4207	O	LEU	544	55.451	56.053	52.400	1.00	23.44	A	O
ATOM	4208	N	ASP	545	53.477	55.049	51.962	1.00	21.43	A	N
ATOM	4209	CA	ASP	545	53.595	55.075	50.508	1.00	20.10	A	C
ATOM	4210	CB	ASP	545	52.570	54.132	49.902	1.00	20.20	A	C
ATOM	4211	CG	ASP	545	52.826	53.848	48.444	1.00	20.73	A	C
ATOM	4212	OD1	ASP	545	53.175	54.790	47.699	1.00	22.69	A	O
ATOM	4213	OD2	ASP	545	52.660	52.675	48.044	1.00	19.91	A	O

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## FIG. 4 - 87

(Continued)

ATOM	4214	C	ASP	545	53.281	56.499	50.078	1.00	20.41	A	C
ATOM	4215	O	ASP	545	52.149	56.949	50.219	1.00	21.14	A	O
ATOM	4216	N	VAL	546	54.263	57.201	49.524	1.00	19.56	A	N
ATOM	4217	CA	VAL	546	54.043	58.591	49.157	1.00	20.20	A	C
ATOM	4218	CB	VAL	546	54.867	59.511	50.090	1.00	20.60	A	C
ATOM	4219	CG1	VAL	546	54.626	60.966	49.753	1.00	20.01	A	C
ATOM	4220	CG2	VAL	546	54.499	59.239	51.533	1.00	21.16	A	C
ATOM	4221	C	VAL	546	54.320	59.032	47.723	1.00	20.28	A	C
ATOM	4222	O	VAL	546	55.212	58.513	47.048	1.00	22.79	A	O
ATOM	4223	N	TYR	547	53.524	59.994	47.267	1.00	17.64	A	N
ATOM	4224	CA	TYR	547	53.702	60.604	45.957	1.00	15.73	A	C
ATOM	4225	CB	TYR	547	52.653	60.155	44.952	1.00	13.49	A	C
ATOM	4226	CG	TYR	547	52.969	60.718	43.589	1.00	13.89	A	C
ATOM	4227	CD1	TYR	547	52.160	61.688	43.006	1.00	14.20	A	C
ATOM	4228	CE1	TYR	547	52.513	62.274	41.801	1.00	13.67	A	C
ATOM	4229	CD2	TYR	547	54.136	60.347	42.921	1.00	9.92	A	C
ATOM	4230	CE2	TYR	547	54.492	60.926	41.726	1.00	10.35	A	C
ATOM	4231	CZ	TYR	547	53.680	61.890	41.167	1.00	12.20	A	C
ATOM	4232	OH	TYR	547	54.036	62.474	39.973	1.00	14.66	A	O
ATOM	4233	C	TYR	547	53.522	62.076	46.266	1.00	14.99	A	C
ATOM	4234	O	TYR	547	54.490	62.834	46.325	1.00	14.47	A	O
ATOM	4235	N	ALA	548	52.265	62.456	46.479	1.00	14.77	A	N
ATOM	4236	CA	ALA	548	51.879	63.806	46.878	1.00	12.10	A	C
ATOM	4237	CB	ALA	548	52.493	64.109	48.247	1.00	9.78	A	C
ATOM	4238	C	ALA	548	52.163	64.950	45.923	1.00	11.87	A	C
ATOM	4239	O	ALA	548	52.250	66.094	46.346	1.00	12.24	A	O
ATOM	4240	N	GLY	549	52.308	64.660	44.639	1.00	13.59	A	N
ATOM	4241	CA	GLY	549	52.556	65.734	43.696	1.00	13.20	A	C
ATOM	4242	C	GLY	549	51.306	66.578	43.573	1.00	13.15	A	C
ATOM	4243	O	GLY	549	50.266	66.182	44.074	1.00	12.86	A	O
ATOM	4244	N	PRO	550	51.365	67.745	42.915	1.00	15.91	A	N
ATOM	4245	CD	PRO	550	52.533	68.380	42.280	1.00	16.15	A	C
ATOM	4246	CA	PRO	550	50.174	68.592	42.776	1.00	15.03	A	C
ATOM	4247	CB	PRO	550	50.693	69.794	41.989	1.00	15.29	A	C
ATOM	4248	CG	PRO	550	52.145	69.838	42.325	1.00	15.06	A	C
ATOM	4249	C	PRO	550	49.074	67.848	42.026	1.00	15.37	A	C
ATOM	4250	O	PRO	550	49.336	67.204	41.012	1.00	16.91	A	O
ATOM	4251	N	CYS	551	47.849	67.946	42.532	1.00	15.67	A	N
ATOM	4252	CA	CYS	551	46.684	67.287	41.944	1.00	16.54	A	C
ATOM	4253	CB	CYS	551	46.424	67.796	40.525	1.00	16.53	A	C
ATOM	4254	SG	CYS	551	44.792	67.314	39.844	1.00	18.29	A	S
ATOM	4255	C	CYS	551	46.811	65.766	41.925	1.00	16.83	A	C
ATOM	4256	O	CYS	551	46.228	65.096	41.087	1.00	20.00	A	O
ATOM	4257	N	SER	552	47.574	65.219	42.856	1.00	16.56	A	N
ATOM	4258	CA	SER	552	47.742	63.785	42.933	1.00	16.35	A	C
ATOM	4259	CB	SER	552	49.063	63.450	43.613	1.00	19.76	A	C
ATOM	4260	OG	SER	552	49.023	63.805	44.987	1.00	20.36	A	O
ATOM	4261	C	SER	552	46.602	63.202	43.760	1.00	17.72	A	C
ATOM	4262	O	SER	552	45.723	63.929	44.243	1.00	17.55	A	O

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(Continued)

## FIG. 4 - 88

ATOM	4263	N	GLN	553	46.632	61.885	43.926	1.00	17.07	A	N
ATOM	4264	CA	GLN	553	45.628	61.179	44.699	1.00	16.87	A	C
ATOM	4265	CB	GLN	553	44.301	61.090	43.937	1.00	16.43	A	C
ATOM	4266	CG	GLN	553	43.249	60.292	44.695	1.00	19.53	A	C
ATOM	4267	CD	GLN	553	41.844	60.468	44.163	1.00	18.87	A	C
ATOM	4268	OE1	GLN	553	41.520	60.019	43.066	1.00	20.67	A	O
ATOM	4269	NE2	GLN	553	40.999	61.126	44.944	1.00	18.67	A	N
ATOM	4270	C	GLN	553	46.123	59.781	44.996	1.00	18.09	A	C
ATOM	4271	O	GLN	553	46.088	58.915	44.129	1.00	18.25	A	O
ATOM	4272	N	LYS	554	46.589	59.562	46.221	1.00	19.53	A	N
ATOM	4273	CA	LYS	554	47.075	58.248	46.620	1.00	20.69	A	C
ATOM	4274	CB	LYS	554	48.319	58.387	47.490	1.00	22.65	A	C
ATOM	4275	CG	LYS	554	49.538	58.887	46.733	1.00	24.15	A	C
ATOM	4276	CD	LYS	554	50.064	57.840	45.765	1.00	25.21	A	C
ATOM	4277	CE	LYS	554	50.777	56.711	46.503	1.00	24.75	A	C
ATOM	4278	NZ	LYS	554	51.472	55.796	45.560	1.00	23.89	A	N
ATOM	4279	C	LYS	554	45.996	57.472	47.374	1.00	21.48	A	C
ATOM	4280	O	LYS	554	46.108	56.258	47.549	1.00	22.39	A	O
ATOM	4281	N	ALA	555	44.952	58.176	47.807	1.00	20.77	A	N
ATOM	4282	CA	ALA	555	43.849	57.555	48.538	1.00	20.46	A	C
ATOM	4283	CB	ALA	555	43.525	58.376	49.768	1.00	18.05	A	C
ATOM	4284	C	ALA	555	42.611	57.436	47.643	1.00	21.32	A	C
ATOM	4285	O	ALA	555	41.996	58.442	47.285	1.00	21.75	A	O
ATOM	4286	N	ASP	556	42.249	56.208	47.283	1.00	21.00	A	N
ATOM	4287	CA	ASP	556	41.096	55.981	46.419	1.00	20.04	A	C
ATOM	4288	CB	ASP	556	41.500	56.151	44.960	1.00	20.02	A	C
ATOM	4289	CG	ASP	556	42.649	55.255	44.574	1.00	19.76	A	C
ATOM	4290	OD1	ASP	556	42.723	54.132	45.115	1.00	19.65	A	O
ATOM	4291	OD2	ASP	556	43.470	55.666	43.723	1.00	21.90	A	O
ATOM	4292	C	ASP	556	40.478	54.603	46.614	1.00	20.18	A	C
ATOM	4293	O	ASP	556	40.856	53.874	47.523	1.00	19.93	A	O
ATOM	4294	N	THR	557	39.542	54.246	45.736	1.00	20.55	A	N
ATOM	4295	CA	THR	557	38.835	52.965	45.820	1.00	22.31	A	C
ATOM	4296	CB	THR	557	37.331	53.154	45.578	1.00	21.37	A	C
ATOM	4297	OG1	THR	557	37.130	53.580	44.224	1.00	21.50	A	O
ATOM	4298	CG2	THR	557	36.754	54.201	46.523	1.00	21.28	A	C
ATOM	4299	C	THR	557	39.294	51.898	44.826	1.00	23.72	A	C
ATOM	4300	O	THR	557	38.606	50.891	44.633	1.00	25.32	A	O
ATOM	4301	N	VAL	558	40.441	52.105	44.194	1.00	22.84	A	N
ATOM	4302	CA	VAL	558	40.931	51.143	43.219	1.00	22.53	A	C
ATOM	4303	CB	VAL	558	41.970	51.802	42.294	1.00	22.67	A	C
ATOM	4304	CG1	VAL	558	42.540	50.783	41.323	1.00	19.20	A	C
ATOM	4305	CG2	VAL	558	41.323	52.964	41.547	1.00	21.12	A	C
ATOM	4306	C	VAL	558	41.544	49.906	43.871	1.00	23.92	A	C
ATOM	4307	O	VAL	558	42.246	50.005	44.871	1.00	23.71	A	O
ATOM	4308	N	PHE	559	41.261	48.734	43.312	1.00	25.05	A	N
ATOM	4309	CA	PHE	559	41.815	47.492	43.841	1.00	25.45	A	C
ATOM	4310	CB	PHE	559	40.855	46.326	43.584	1.00	24.60	A	C
ATOM	4311	CG	PHE	559	41.476	44.977	43.808	1.00	24.75	A	C

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(Continued)

## F I G. 4 - 8 9

ATOM	4312	CD1	PHE	559	42.192	44.352	42.799	1.00	25.70	A	C
ATOM	4313	CD2	PHE	559	41.382	44.352	45.044	1.00	25.27	A	C
ATOM	4314	CE1	PHE	559	42.810	43.118	43.021	1.00	28.04	A	C
ATOM	4315	CE2	PHE	559	41.995	43.125	45.276	1.00	24.71	A	C
ATOM	4316	CZ	PHE	559	42.709	42.507	44.266	1.00	26.38	A	C
ATOM	4317	C	PHE	559	43.158	47.210	43.170	1.00	26.14	A	C
ATOM	4318	O	PHE	559	43.250	47.246	41.943	1.00	27.21	A	O
ATOM	4319	N	ARG	560	44.188	46.912	43.962	1.00	24.72	A	N
ATOM	4320	CA	ARG	560	45.508	46.644	43.397	1.00	23.52	A	C
ATOM	4321	CB	ARG	560	46.398	47.892	43.510	1.00	20.68	A	C
ATOM	4322	CG	ARG	560	45.869	49.140	42.802	1.00	19.21	A	C
ATOM	4323	CD	ARG	560	46.885	50.285	42.869	1.00	17.64	A	C
ATOM	4324	NE	ARG	560	46.269	51.536	43.310	1.00	20.38	A	N
ATOM	4325	CZ	ARG	560	45.637	52.391	42.515	1.00	20.51	A	C
ATOM	4326	NH1	ARG	560	45.543	52.149	41.218	1.00	26.51	A	N
ATOM	4327	NH2	ARG	560	45.061	53.468	43.022	1.00	20.25	A	N
ATOM	4328	C	ARG	560	46.274	45.451	43.980	1.00	24.37	A	C
ATOM	4329	O	ARG	560	46.112	45.081	45.145	1.00	24.84	A	O
ATOM	4330	N	LEU	561	47.111	44.856	43.136	1.00	23.62	A	N
ATOM	4331	CA	LEU	561	47.968	43.740	43.511	1.00	20.95	A	C
ATOM	4332	CB	LEU	561	47.680	42.523	42.635	1.00	18.87	A	C
ATOM	4333	CG	LEU	561	46.283	41.916	42.773	1.00	20.60	A	C
ATOM	4334	CD1	LEU	561	46.139	40.749	41.803	1.00	19.75	A	C
ATOM	4335	CD2	LEU	561	46.045	41.460	44.203	1.00	17.53	A	C
ATOM	4336	C	LEU	561	49.380	44.255	43.246	1.00	20.00	A	C
ATOM	4337	O	LEU	561	49.894	44.152	42.133	1.00	20.19	A	O
ATOM	4338	N	ASN	562	49.999	44.822	44.274	1.00	18.97	A	N
ATOM	4339	CA	ASN	562	51.335	45.392	44.142	1.00	18.20	A	C
ATOM	4340	CB	ASN	562	51.197	46.907	44.028	1.00	16.72	A	C
ATOM	4341	CG	ASN	562	50.364	47.491	45.148	1.00	17.45	A	C
ATOM	4342	OD1	ASN	562	49.881	48.610	45.054	1.00	19.63	A	O
ATOM	4343	ND2	ASN	562	50.195	46.729	46.223	1.00	18.39	A	N
ATOM	4344	C	ASN	562	52.291	45.035	45.289	1.00	18.48	A	C
ATOM	4345	O	ASN	562	52.055	44.098	46.056	1.00	19.79	A	O
ATOM	4346	N	TRP	563	53.375	45.793	45.400	1.00	17.98	A	N
ATOM	4347	CA	TRP	563	54.366	45.548	46.434	1.00	17.62	A	C
ATOM	4348	CB	TRP	563	55.538	46.537	46.290	1.00	16.04	A	C
ATOM	4349	CG	TRP	563	56.741	46.249	47.178	1.00	15.76	A	C
ATOM	4350	CD2	TRP	563	57.474	47.200	47.968	1.00	13.80	A	C
ATOM	4351	CE2	TRP	563	58.526	46.500	48.602	1.00	11.13	A	C
ATOM	4352	CE3	TRP	563	57.341	48.575	48.198	1.00	13.46	A	C
ATOM	4353	CD1	TRP	563	57.367	45.041	47.361	1.00	12.65	A	C
ATOM	4354	NE1	TRP	563	58.440	45.189	48.217	1.00	11.34	A	N
ATOM	4355	CZ2	TRP	563	59.439	47.128	49.453	1.00	14.40	A	C
ATOM	4356	CZ3	TRP	563	58.252	49.204	49.046	1.00	16.29	A	C
ATOM	4357	CH2	TRP	563	59.291	48.476	49.664	1.00	14.18	A	C
ATOM	4358	C	TRP	563	53.728	45.672	47.809	1.00	17.48	A	C
ATOM	4359	O	TRP	563	54.048	44.910	48.720	1.00	18.93	A	O
ATOM	4360	N	ALA	564	52.813	46.620	47.953	1.00	16.80	A	N

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(Continued)

## FIG. 4 - 90

ATOM	4361	CA	ALA	564	52.151	46.838	49.232	1.00	17.11	A	C
ATOM	4362	CB	ALA	564	51.248	48.068	49.153	1.00	16.72	A	C
ATOM	4363	C	ALA	564	51.341	45.616	49.655	1.00	17.89	A	C
ATOM	4364	O	ALA	564	51.322	45.256	50.834	1.00	15.94	A	O
ATOM	4365	N	THR	565	50.676	44.983	48.691	1.00	18.77	A	N
ATOM	4366	CA	THR	565	49.870	43.801	48.977	1.00	19.59	A	C
ATOM	4367	CB	THR	565	49.368	43.131	47.689	1.00	20.01	A	C
ATOM	4368	OG1	THR	565	48.606	44.069	46.922	1.00	19.76	A	O
ATOM	4369	CG2	THR	565	48.496	41.922	48.027	1.00	19.34	A	C
ATOM	4370	C	THR	565	50.718	42.793	49.739	1.00	21.27	A	C
ATOM	4371	O	THR	565	50.290	42.252	50.760	1.00	22.29	A	O
ATOM	4372	N	TYR	566	51.924	42.548	49.234	1.00	22.25	A	N
ATOM	4373	CA	TYR	566	52.848	41.615	49.864	1.00	23.40	A	C
ATOM	4374	CB	TYR	566	54.029	41.324	48.923	1.00	25.18	A	C
ATOM	4375	CG	TYR	566	55.369	41.218	49.616	1.00	25.40	A	C
ATOM	4376	CD1	TYR	566	56.297	42.262	49.547	1.00	25.62	A	C
ATOM	4377	CE1	TYR	566	57.513	42.196	50.226	1.00	26.85	A	C
ATOM	4378	CD2	TYR	566	55.690	40.101	50.382	1.00	26.99	A	C
ATOM	4379	CE2	TYR	566	56.903	40.023	51.073	1.00	29.74	A	C
ATOM	4380	CZ	TYR	566	57.809	41.074	50.991	1.00	30.16	A	C
ATOM	4381	OH	TYR	566	58.997	40.998	51.688	1.00	32.61	A	O
ATOM	4382	C	TYR	566	53.369	42.116	51.212	1.00	23.06	A	C
ATOM	4383	O	TYR	566	53.458	41.350	52.170	1.00	21.96	A	O
ATOM	4384	N	LEU	567	53.716	43.396	51.288	1.00	23.28	A	N
ATOM	4385	CA	LEU	567	54.237	43.949	52.532	1.00	24.50	A	C
ATOM	4386	CB	LEU	567	54.588	45.429	52.359	1.00	22.74	A	C
ATOM	4387	CG	LEU	567	55.717	45.769	51.378	1.00	23.15	A	C
ATOM	4388	CD1	LEU	567	55.833	47.279	51.263	1.00	20.37	A	C
ATOM	4389	CD2	LEU	567	57.038	45.158	51.850	1.00	21.42	A	C
ATOM	4390	C	LEU	567	53.243	43.786	53.675	1.00	26.32	A	C
ATOM	4391	O	LEU	567	53.635	43.595	54.824	1.00	27.44	A	O
ATOM	4392	N	ALA	568	51.955	43.857	53.361	1.00	26.96	A	N
ATOM	4393	CA	ALA	568	50.930	43.712	54.383	1.00	27.44	A	C
ATOM	4394	CB	ALA	568	49.684	44.481	53.984	1.00	26.54	A	C
ATOM	4395	C	ALA	568	50.584	42.242	54.606	1.00	29.12	A	C
ATOM	4396	O	ALA	568	50.483	41.782	55.748	1.00	28.80	A	O
ATOM	4397	N	SER	569	50.417	41.506	53.509	1.00	28.58	A	N
ATOM	4398	CA	SER	569	50.062	40.094	53.586	1.00	28.31	A	C
ATOM	4399	CB	SER	569	49.750	39.553	52.191	1.00	28.85	A	C
ATOM	4400	OG	SER	569	49.420	38.174	52.247	1.00	30.69	A	O
ATOM	4401	C	SER	569	51.110	39.204	54.236	1.00	27.43	A	C
ATOM	4402	O	SER	569	50.800	38.427	55.133	1.00	28.44	A	O
ATOM	4403	N	THR	570	52.350	39.311	53.781	1.00	27.24	A	N
ATOM	4404	CA	THR	570	53.420	38.483	54.314	1.00	27.02	A	C
ATOM	4405	CB	THR	570	54.410	38.094	53.199	1.00	26.90	A	C
ATOM	4406	OG1	THR	570	53.749	37.250	52.248	1.00	27.63	A	O
ATOM	4407	CG2	THR	570	55.611	37.369	53.774	1.00	23.88	A	C
ATOM	4408	C	THR	570	54.203	39.110	55.459	1.00	27.34	A	C
ATOM	4409	O	THR	570	54.362	38.496	56.512	1.00	30.01	A	O

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## FIG. 4 - 9 1

(Continued)

ATOM	4410	N	GLU	571	54.686	40.329	55.253	1.00	26.71	A	N
ATOM	4411	CA	GLU	571	55.480	41.020	56.259	1.00	25.23	A	C
ATOM	4412	CB	GLU	571	56.402	42.040	55.583	1.00	24.64	A	C
ATOM	4413	CG	GLU	571	57.287	41.472	54.473	1.00	25.43	A	C
ATOM	4414	CD	GLU	571	58.238	40.392	54.966	1.00	27.45	A	C
ATOM	4415	OE1	GLU	571	58.582	40.421	56.164	1.00	28.11	A	O
ATOM	4416	OE2	GLU	571	58.656	39.527	54.158	1.00	27.18	A	O
ATOM	4417	C	GLU	571	54.643	41.715	57.329	1.00	24.50	A	C
ATOM	4418	O	GLU	571	55.188	42.368	58.213	1.00	24.29	A	O
ATOM	4419	N	ASN	572	53.324	41.576	57.247	1.00	24.39	A	N
ATOM	4420	CA	ASN	572	52.425	42.191	58.223	1.00	24.96	A	C
ATOM	4421	CB	ASN	572	52.557	41.486	59.569	1.00	25.44	A	C
ATOM	4422	CG	ASN	572	52.139	40.033	59.507	1.00	29.03	A	C
ATOM	4423	OD1	ASN	572	52.711	39.187	60.192	1.00	30.88	A	O
ATOM	4424	ND2	ASN	572	51.128	39.734	58.694	1.00	29.67	A	N
ATOM	4425	C	ASN	572	52.683	43.681	58.419	1.00	25.32	A	C
ATOM	4426	O	ASN	572	52.642	44.178	59.545	1.00	25.55	A	O
ATOM	4427	N	ILE	573	52.944	44.387	57.321	1.00	25.48	A	N
ATOM	4428	CA	ILE	573	53.208	45.824	57.360	1.00	24.87	A	C
ATOM	4429	CB	ILE	573	54.396	46.198	56.446	1.00	24.59	A	C
ATOM	4430	CG2	ILE	573	54.715	47.669	56.584	1.00	22.90	A	C
ATOM	4431	CG1	ILE	573	55.622	45.365	56.800	1.00	25.08	A	C
ATOM	4432	CD1	ILE	573	56.805	45.636	55.900	1.00	25.36	A	C
ATOM	4433	C	ILE	573	51.992	46.621	56.875	1.00	25.22	A	C
ATOM	4434	O	ILE	573	51.353	46.249	55.891	1.00	24.86	A	O
ATOM	4435	N	ILE	574	51.681	47.718	57.557	1.00	24.59	A	N
ATOM	4436	CA	ILE	574	50.557	48.555	57.159	1.00	26.14	A	C
ATOM	4437	CB	ILE	574	49.926	49.297	58.359	1.00	25.88	A	C
ATOM	4438	CG2	ILE	574	48.798	50.190	57.874	1.00	26.06	A	C
ATOM	4439	CG1	ILE	574	49.399	48.304	59.386	1.00	27.36	A	C
ATOM	4440	CD1	ILE	574	48.794	48.968	60.607	1.00	29.19	A	C
ATOM	4441	C	ILE	574	51.064	49.619	56.191	1.00	27.12	A	C
ATOM	4442	O	ILE	574	51.799	50.524	56.591	1.00	28.97	A	O
ATOM	4443	N	VAL	575	50.683	49.521	54.924	1.00	25.92	A	N
ATOM	4444	CA	VAL	575	51.128	50.517	53.962	1.00	24.87	A	C
ATOM	4445	CB	VAL	575	51.387	49.904	52.569	1.00	24.76	A	C
ATOM	4446	CG1	VAL	575	51.973	50.966	51.644	1.00	20.17	A	C
ATOM	4447	CG2	VAL	575	52.320	48.707	52.690	1.00	22.12	A	C
ATOM	4448	C	VAL	575	50.054	51.585	53.837	1.00	25.21	A	C
ATOM	4449	O	VAL	575	48.929	51.312	53.405	1.00	25.63	A	O
ATOM	4450	N	ALA	576	50.403	52.804	54.216	1.00	23.75	A	N
ATOM	4451	CA	ALA	576	49.456	53.893	54.152	1.00	23.56	A	C
ATOM	4452	CB	ALA	576	49.255	54.477	55.540	1.00	23.43	A	C
ATOM	4453	C	ALA	576	49.879	54.988	53.180	1.00	24.06	A	C
ATOM	4454	O	ALA	576	51.056	55.139	52.860	1.00	22.16	A	O
ATOM	4455	N	SER	577	48.888	55.740	52.710	1.00	24.49	A	N
ATOM	4456	CA	SER	577	49.095	56.852	51.796	1.00	23.11	A	C
ATOM	4457	CB	SER	577	48.793	56.428	50.362	1.00	23.06	A	C
ATOM	4458	OG	SER	577	49.750	55.475	49.921	1.00	22.88	A	O

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(Continued)

## FIG. 4 - 9 2

ATOM	4459	C	SER	577	48.149	57.947	52.248	1.00	22.90	A	C
ATOM	4460	O	SER	577	47.075	57.662	52.768	1.00	24.22	A	O
ATOM	4461	N	PHE	578	48.546	59.196	52.046	1.00	23.49	A	N
ATOM	4462	CA	PHE	578	47.748	60.337	52.479	1.00	21.77	A	C
ATOM	4463	CB	PHE	578	48.313	60.829	53.804	1.00	21.41	A	C
ATOM	4464	CG	PHE	578	47.585	62.005	54.383	1.00	22.79	A	C
ATOM	4465	CD1	PHE	578	46.429	61.820	55.144	1.00	20.60	A	C
ATOM	4466	CD2	PHE	578	48.080	63.291	54.209	1.00	19.79	A	C
ATOM	4467	CE1	PHE	578	45.783	62.901	55.730	1.00	21.26	A	C
ATOM	4468	CE2	PHE	578	47.441	64.381	54.790	1.00	20.94	A	C
ATOM	4469	CZ	PHE	578	46.288	64.186	55.556	1.00	20.70	A	C
ATOM	4470	C	PHE	578	47.723	61.502	51.480	1.00	21.14	A	C
ATOM	4471	O	PHE	578	48.766	61.909	50.973	1.00	21.08	A	O
ATOM	4472	N	ASP	579	46.533	62.041	51.212	1.00	19.89	A	N
ATOM	4473	CA	ASP	579	46.389	63.173	50.302	1.00	18.01	A	C
ATOM	4474	CB	ASP	579	45.191	62.985	49.371	1.00	17.01	A	C
ATOM	4475	CG	ASP	579	45.334	61.777	48.455	1.00	21.86	A	C
ATOM	4476	OD1	ASP	579	46.424	61.583	47.873	1.00	22.87	A	O
ATOM	4477	OD2	ASP	579	44.342	61.024	48.299	1.00	23.17	A	O
ATOM	4478	C	ASP	579	46.211	64.474	51.092	1.00	18.10	A	C
ATOM	4479	O	ASP	579	45.103	64.823	51.493	1.00	20.42	A	O
ATOM	4480	N	GLY	580	47.306	65.189	51.313	1.00	17.22	A	N
ATOM	4481	CA	GLY	580	47.238	66.439	52.044	1.00	15.14	A	C
ATOM	4482	C	GLY	580	47.065	67.610	51.098	1.00	16.53	A	C
ATOM	4483	O	GLY	580	46.544	67.462	49.993	1.00	17.18	A	O
ATOM	4484	N	ARG	581	47.495	68.786	51.528	1.00	15.90	A	N
ATOM	4485	CA	ARG	581	47.377	69.970	50.701	1.00	15.52	A	C
ATOM	4486	CB	ARG	581	47.956	71.172	51.444	1.00	16.17	A	C
ATOM	4487	CG	ARG	581	47.072	71.645	52.585	1.00	16.05	A	C
ATOM	4488	CD	ARG	581	47.756	72.653	53.467	1.00	14.87	A	C
ATOM	4489	NE	ARG	581	48.617	71.990	54.441	1.00	18.25	A	N
ATOM	4490	CZ	ARG	581	49.321	72.624	55.375	1.00	19.44	A	C
ATOM	4491	NH1	ARG	581	49.268	73.952	55.463	1.00	20.41	A	N
ATOM	4492	NH2	ARG	581	50.075	71.933	56.224	1.00	15.76	A	N
ATOM	4493	C	ARG	581	48.107	69.742	49.386	1.00	17.75	A	C
ATOM	4494	O	ARG	581	49.193	69.158	49.357	1.00	17.49	A	O
ATOM	4495	N	GLY	582	47.495	70.192	48.295	1.00	18.96	A	N
ATOM	4496	CA	GLY	582	48.094	70.022	46.987	1.00	17.63	A	C
ATOM	4497	C	GLY	582	47.511	68.842	46.231	1.00	18.54	A	C
ATOM	4498	O	GLY	582	47.673	68.757	45.017	1.00	18.99	A	O
ATOM	4499	N	SER	583	46.842	67.923	46.925	1.00	18.00	A	N
ATOM	4500	CA	SER	583	46.258	66.765	46.247	1.00	18.46	A	C
ATOM	4501	CB	SER	583	45.842	65.700	47.269	1.00	18.34	A	C
ATOM	4502	OG	SER	583	45.058	66.253	48.303	1.00	19.12	A	O
ATOM	4503	C	SER	583	45.068	67.218	45.392	1.00	18.03	A	C
ATOM	4504	O	SER	583	44.601	68.344	45.536	1.00	17.42	A	O
ATOM	4505	N	GLY	584	44.570	66.355	44.510	1.00	17.84	A	N
ATOM	4506	CA	GLY	584	43.481	66.779	43.637	1.00	19.22	A	C
ATOM	4507	C	GLY	584	42.052	66.293	43.827	1.00	19.49	A	C

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## FIG. 4 - 93

(Continued)

ATOM	4508	O	GLY	584	41.724	65.570	44.767	1.00	21.57	A	O
ATOM	4509	N	TYR	585	41.191	66.735	42.917	1.00	19.76	A	N
ATOM	4510	CA	TYR	585	39.782	66.362	42.906	1.00	18.53	A	C
ATOM	4511	CB	TYR	585	39.673	64.859	42.663	1.00	18.57	A	C
ATOM	4512	CG	TYR	585	40.578	64.401	41.550	1.00	18.83	A	C
ATOM	4513	CD1	TYR	585	40.439	64.914	40.260	1.00	19.48	A	C
ATOM	4514	CE1	TYR	585	41.300	64.533	39.235	1.00	18.11	A	C
ATOM	4515	CD2	TYR	585	41.606	63.490	41.789	1.00	19.81	A	C
ATOM	4516	CE2	TYR	585	42.476	63.100	40.769	1.00	17.71	A	C
ATOM	4517	CZ	TYR	585	42.313	63.626	39.497	1.00	18.76	A	C
ATOM	4518	OH	TYR	585	43.150	63.232	38.481	1.00	20.70	A	O
ATOM	4519	C	TYR	585	38.997	66.751	44.152	1.00	18.81	A	C
ATOM	4520	O	TYR	585	38.046	66.067	44.521	1.00	17.85	A	O
ATOM	4521	N	GLN	586	39.382	67.861	44.783	1.00	20.25	A	N
ATOM	4522	CA	GLN	586	38.708	68.345	45.986	1.00	20.04	A	C
ATOM	4523	CB	GLN	586	39.455	67.886	47.233	1.00	20.09	A	C
ATOM	4524	CG	GLN	586	39.770	66.412	47.279	1.00	20.60	A	C
ATOM	4525	CD	GLN	586	40.781	66.095	48.363	1.00	24.77	A	C
ATOM	4526	OE1	GLN	586	40.441	66.029	49.548	1.00	23.60	A	O
ATOM	4527	NE2	GLN	586	42.044	65.919	47.962	1.00	25.12	A	N
ATOM	4528	C	GLN	586	38.619	69.869	46.024	1.00	22.06	A	C
ATOM	4529	O	GLN	586	38.424	70.455	47.092	1.00	23.83	A	O
ATOM	4530	N	GLY	587	38.783	70.518	44.877	1.00	21.79	A	N
ATOM	4531	CA	GLY	587	38.707	71.969	44.853	1.00	21.24	A	C
ATOM	4532	C	GLY	587	40.073	72.623	44.883	1.00	21.56	A	C
ATOM	4533	O	GLY	587	41.033	72.035	45.364	1.00	23.11	A	O
ATOM	4534	N	ASP	588	40.154	73.856	44.397	1.00	21.25	A	N
ATOM	4535	CA	ASP	588	41.415	74.580	44.339	1.00	22.09	A	C
ATOM	4536	CB	ASP	588	41.287	75.763	43.382	1.00	22.35	A	C
ATOM	4537	CG	ASP	588	40.944	75.340	41.965	1.00	25.14	A	C
ATOM	4538	OD1	ASP	588	40.465	76.213	41.211	1.00	25.77	A	O
ATOM	4539	OD2	ASP	588	41.157	74.155	41.599	1.00	24.41	A	O
ATOM	4540	C	ASP	588	41.955	75.079	45.675	1.00	23.08	A	C
ATOM	4541	O	ASP	588	43.121	75.471	45.762	1.00	22.71	A	O
ATOM	4542	N	LYS	589	41.130	75.086	46.716	1.00	23.77	A	N
ATOM	4543	CA	LYS	589	41.620	75.562	47.998	1.00	22.97	A	C
ATOM	4544	CB	LYS	589	40.509	75.616	49.037	1.00	24.26	A	C
ATOM	4545	CG	LYS	589	40.994	76.173	50.365	1.00	29.68	A	C
ATOM	4546	CD	LYS	589	39.916	76.141	51.439	1.00	35.08	A	C
ATOM	4547	CE	LYS	589	40.457	76.638	52.784	1.00	36.09	A	C
ATOM	4548	NZ	LYS	589	39.461	76.464	53.881	1.00	36.83	A	N
ATOM	4549	C	LYS	589	42.705	74.611	48.468	1.00	22.93	A	C
ATOM	4550	O	LYS	589	43.711	75.032	49.033	1.00	23.71	A	O
ATOM	4551	N	ILE	590	42.494	73.326	48.217	1.00	21.82	A	N
ATOM	4552	CA	ILE	590	43.444	72.302	48.607	1.00	21.76	A	C
ATOM	4553	CB	ILE	590	42.737	70.956	48.846	1.00	20.55	A	C
ATOM	4554	CG2	ILE	590	43.756	69.841	48.934	1.00	19.40	A	C
ATOM	4555	CG1	ILE	590	41.901	71.025	50.126	1.00	21.94	A	C
ATOM	4556	CD1	ILE	590	41.200	69.720	50.478	1.00	22.22	A	C

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(Continued)

## FIG. 4 - 94

ATOM	4557	C	ILE	590	44.537	72.093	47.562	1.00	22.32	A	C
ATOM	4558	O	ILE	590	45.711	71.960	47.901	1.00	23.51	A	O
ATOM	4559	N	MET	591	44.157	72.071	46.291	1.00	21.59	A	N
ATOM	4560	CA	MET	591	45.127	71.846	45.232	1.00	21.59	A	C
ATOM	4561	CB	MET	591	44.406	71.567	43.917	1.00	21.80	A	C
ATOM	4562	CG	MET	591	45.309	71.000	42.838	1.00	21.85	A	C
ATOM	4563	SD	MET	591	44.403	70.746	41.309	1.00	22.76	A	S
ATOM	4564	CE	MET	591	44.237	72.436	40.732	1.00	22.84	A	C
ATOM	4565	C	MET	591	46.112	72.997	45.051	1.00	21.43	A	C
ATOM	4566	O	MET	591	47.289	72.771	44.791	1.00	19.25	A	O
ATOM	4567	N	HIS	592	45.636	74.228	45.200	1.00	21.21	A	N
ATOM	4568	CA	HIS	592	46.502	75.386	45.035	1.00	21.43	A	C
ATOM	4569	CB	HIS	592	45.713	76.560	44.455	1.00	22.32	A	C
ATOM	4570	CG	HIS	592	45.296	76.361	43.032	1.00	24.65	A	C
ATOM	4571	CD2	HIS	592	45.604	75.390	42.139	1.00	26.25	A	C
ATOM	4572	ND1	HIS	592	44.471	77.243	42.368	1.00	25.75	A	N
ATOM	4573	CE1	HIS	592	44.289	76.825	41.128	1.00	25.99	A	C
ATOM	4574	NE2	HIS	592	44.965	75.703	40.962	1.00	25.78	A	N
ATOM	4575	C	HIS	592	47.197	75.817	46.319	1.00	21.38	A	C
ATOM	4576	O	HIS	592	47.842	76.865	46.362	1.00	20.84	A	O
ATOM	4577	N	ALA	593	47.076	75.012	47.367	1.00	21.76	A	N
ATOM	4578	CA	ALA	593	47.732	75.349	48.628	1.00	20.43	A	C
ATOM	4579	CB	ALA	593	47.360	74.349	49.710	1.00	18.24	A	C
ATOM	4580	C	ALA	593	49.241	75.361	48.427	1.00	19.92	A	C
ATOM	4581	O	ALA	593	49.940	76.126	49.081	1.00	21.91	A	O
ATOM	4582	N	ILE	594	49.736	74.522	47.518	1.00	19.47	A	N
ATOM	4583	CA	ILE	594	51.176	74.446	47.248	1.00	20.49	A	C
ATOM	4584	CB	ILE	594	51.617	73.021	46.816	1.00	19.36	A	C
ATOM	4585	CG2	ILE	594	51.467	72.051	47.966	1.00	19.38	A	C
ATOM	4586	CG1	ILE	594	50.814	72.581	45.590	1.00	21.33	A	C
ATOM	4587	CD1	ILE	594	50.951	71.106	45.243	1.00	22.55	A	C
ATOM	4588	C	ILE	594	51.658	75.410	46.169	1.00	19.88	A	C
ATOM	4589	O	ILE	594	52.849	75.434	45.854	1.00	17.79	A	O
ATOM	4590	N	ASN	595	50.746	76.200	45.606	1.00	20.03	A	N
ATOM	4591	CA	ASN	595	51.119	77.137	44.547	1.00	21.76	A	C
ATOM	4592	CB	ASN	595	49.977	78.114	44.265	1.00	20.68	A	C
ATOM	4593	CG	ASN	595	50.300	79.072	43.128	1.00	21.80	A	C
ATOM	4594	OD1	ASN	595	50.640	78.652	42.024	1.00	22.78	A	O
ATOM	4595	ND2	ASN	595	50.191	80.364	43.394	1.00	22.74	A	N
ATOM	4596	C	ASN	595	52.395	77.921	44.860	1.00	22.25	A	C
ATOM	4597	O	ASN	595	52.442	78.688	45.824	1.00	22.44	A	O
ATOM	4598	N	ARG	596	53.421	77.715	44.031	1.00	22.52	A	N
ATOM	4599	CA	ARG	596	54.726	78.378	44.171	1.00	22.41	A	C
ATOM	4600	CB	ARG	596	54.550	79.898	44.141	1.00	21.28	A	C
ATOM	4601	CG	ARG	596	53.894	80.426	42.880	1.00	21.31	A	C
ATOM	4602	CD	ARG	596	53.398	81.856	43.096	1.00	22.01	A	C
ATOM	4603	NE	ARG	596	54.479	82.760	43.482	1.00	20.88	A	N
ATOM	4604	CZ	ARG	596	55.467	83.112	42.671	1.00	21.35	A	C
ATOM	4605	NH1	ARG	596	55.498	82.635	41.431	1.00	22.62	A	N

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## FIG. 4 - 95

(Continued)

ATOM	4606	NH2	ARG	596	56.427	83.924	43.096	1.00	19.92	A	N
ATOM	4607	C	ARG	596	55.492	77.982	45.440	1.00	21.53	A	C
ATOM	4608	O	ARG	596	56.482	78.611	45.804	1.00	20.59	A	O
ATOM	4609	N	ARG	597	55.046	76.930	46.107	1.00	21.66	A	N
ATOM	4610	CA	ARG	597	55.705	76.512	47.331	1.00	21.98	A	C
ATOM	4611	CB	ARG	597	54.943	77.061	48.539	1.00	23.55	A	C
ATOM	4612	CG	ARG	597	55.184	78.547	48.776	1.00	28.20	A	C
ATOM	4613	CD	ARG	597	56.611	78.813	49.264	1.00	30.86	A	C
ATOM	4614	NE	ARG	597	56.891	80.239	49.414	1.00	34.81	A	N
ATOM	4615	CZ	ARG	597	57.074	81.088	48.401	1.00	36.01	A	C
ATOM	4616	NH1	ARG	597	57.011	80.670	47.142	1.00	33.57	A	N
ATOM	4617	NH2	ARG	597	57.326	82.365	48.650	1.00	37.36	A	N
ATOM	4618	C	ARG	597	55.869	75.011	47.458	1.00	20.79	A	C
ATOM	4619	O	ARG	597	55.523	74.423	48.487	1.00	20.19	A	O
ATOM	4620	N	LEU	598	56.400	74.398	46.404	1.00	19.44	A	N
ATOM	4621	CA	LEU	598	56.649	72.963	46.387	1.00	18.48	A	C
ATOM	4622	CB	LEU	598	57.142	72.545	45.003	1.00	18.20	A	C
ATOM	4623	CG	LEU	598	56.119	72.007	43.994	1.00	19.27	A	C
ATOM	4624	CD1	LEU	598	54.800	72.731	44.107	1.00	19.49	A	C
ATOM	4625	CD2	LEU	598	56.691	72.135	42.595	1.00	18.24	A	C
ATOM	4626	C	LEU	598	57.692	72.617	47.450	1.00	19.10	A	C
ATOM	4627	O	LEU	598	58.644	73.363	47.679	1.00	19.27	A	O
ATOM	4628	N	GLY	599	57.506	71.485	48.108	1.00	19.24	A	N
ATOM	4629	CA	GLY	599	58.440	71.090	49.138	1.00	20.34	A	C
ATOM	4630	C	GLY	599	58.055	71.622	50.508	1.00	21.76	A	C
ATOM	4631	O	GLY	599	58.882	71.640	51.422	1.00	23.58	A	O
ATOM	4632	N	THR	600	56.811	72.061	50.666	1.00	21.02	A	N
ATOM	4633	CA	THR	600	56.381	72.578	51.958	1.00	21.20	A	C
ATOM	4634	CB	THR	600	56.039	74.082	51.874	1.00	21.28	A	C
ATOM	4635	OG1	THR	600	54.887	74.271	51.052	1.00	25.68	A	O
ATOM	4636	CG2	THR	600	57.192	74.856	51.264	1.00	21.23	A	C
ATOM	4637	C	THR	600	55.201	71.810	52.557	1.00	21.38	A	C
ATOM	4638	O	THR	600	55.386	70.724	53.100	1.00	22.42	A	O
ATOM	4639	N	PHE	601	53.993	72.356	52.446	1.00	21.18	A	N
ATOM	4640	CA	PHE	601	52.809	71.721	53.022	1.00	22.09	A	C
ATOM	4641	CB	PHE	601	51.540	72.498	52.649	1.00	24.93	A	C
ATOM	4642	CG	PHE	601	51.556	73.935	53.077	1.00	26.21	A	C
ATOM	4643	CD1	PHE	601	51.052	74.923	52.236	1.00	28.07	A	C
ATOM	4644	CD2	PHE	601	52.105	74.308	54.299	1.00	26.83	A	C
ATOM	4645	CE1	PHE	601	51.100	76.271	52.603	1.00	29.10	A	C
ATOM	4646	CE2	PHE	601	52.160	75.650	54.680	1.00	28.02	A	C
ATOM	4647	CZ	PHE	601	51.658	76.636	53.830	1.00	28.61	A	C
ATOM	4648	C	PHE	601	52.623	70.265	52.635	1.00	22.45	A	C
ATOM	4649	O	PHE	601	52.235	69.451	53.470	1.00	22.89	A	O
ATOM	4650	N	GLU	602	52.884	69.931	51.374	1.00	22.76	A	N
ATOM	4651	CA	GLU	602	52.712	68.556	50.931	1.00	21.82	A	C
ATOM	4652	CB	GLU	602	52.956	68.418	49.422	1.00	22.43	A	C
ATOM	4653	CG	GLU	602	54.396	68.559	48.974	1.00	27.44	A	C
ATOM	4654	CD	GLU	602	54.872	70.002	48.893	1.00	29.71	A	C

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## FIG. 4 - 96

(Continued)

ATOM	4655	OE1	GLU	602	54.751	70.743	49.891	1.00	31.66	A	0
ATOM	4656	OE2	GLU	602	55.379	70.392	47.822	1.00	31.46	A	0
ATOM	4657	C	GLU	602	53.663	67.657	51.698	1.00	21.67	A	C
ATOM	4658	O	GLU	602	53.386	66.473	51.899	1.00	22.33	A	0
ATOM	4659	N	VAL	603	54.777	68.229	52.146	1.00	20.78	A	N
ATOM	4660	CA	VAL	603	55.772	67.468	52.897	1.00	20.76	A	C
ATOM	4661	CB	VAL	603	57.159	68.133	52.800	1.00	18.99	A	C
ATOM	4662	CG1	VAL	603	58.165	67.365	53.649	1.00	15.00	A	C
ATOM	4663	CG2	VAL	603	57.603	68.193	51.335	1.00	15.21	A	C
ATOM	4664	C	VAL	603	55.368	67.350	54.364	1.00	21.85	A	C
ATOM	4665	O	VAL	603	55.373	66.265	54.946	1.00	20.44	A	O
ATOM	4666	N	GLU	604	55.009	68.481	54.951	1.00	24.70	A	N
ATOM	4667	CA	GLU	604	54.594	68.518	56.341	1.00	27.84	A	C
ATOM	4668	CB	GLU	604	54.322	69.964	56.770	1.00	30.83	A	C
ATOM	4669	CG	GLU	604	55.572	70.808	56.924	1.00	37.92	A	C
ATOM	4670	CD	GLU	604	56.449	70.355	58.091	1.00	43.63	A	C
ATOM	4671	OE1	GLU	604	57.505	70.989	58.328	1.00	46.30	A	O
ATOM	4672	OE2	GLU	604	56.083	69.368	58.773	1.00	45.85	A	O
ATOM	4673	C	GLU	604	53.349	67.669	56.553	1.00	27.28	A	C
ATOM	4674	O	GLU	604	53.270	66.909	57.517	1.00	28.68	A	O
ATOM	4675	N	ASP	605	52.381	67.786	55.650	1.00	25.92	A	N
ATOM	4676	CA	ASP	605	51.151	67.021	55.785	1.00	25.72	A	C
ATOM	4677	CB	ASP	605	50.144	67.436	54.713	1.00	24.61	A	C
ATOM	4678	CG	ASP	605	49.576	68.832	54.963	1.00	23.36	A	C
ATOM	4679	OD1	ASP	605	48.677	69.267	54.215	1.00	23.15	A	O
ATOM	4680	OD2	ASP	605	50.036	69.499	55.914	1.00	21.27	A	O
ATOM	4681	C	ASP	605	51.379	65.515	55.783	1.00	26.18	A	C
ATOM	4682	O	ASP	605	50.646	64.779	56.439	1.00	28.35	A	O
ATOM	4683	N	GLN	606	52.394	65.051	55.063	1.00	26.16	A	N
ATOM	4684	CA	GLN	606	52.704	63.627	55.056	1.00	25.29	A	C
ATOM	4685	CB	GLN	606	53.788	63.302	54.026	1.00	24.18	A	C
ATOM	4686	CG	GLN	606	53.305	63.332	52.596	1.00	24.92	A	C
ATOM	4687	CD	GLN	606	52.206	62.321	52.330	1.00	24.81	A	C
ATOM	4688	OE1	GLN	606	52.373	61.122	52.560	1.00	25.31	A	O
ATOM	4689	NE2	GLN	606	51.075	62.801	51.840	1.00	25.44	A	N
ATOM	4690	C	GLN	606	53.207	63.268	56.447	1.00	25.47	A	C
ATOM	4691	O	GLN	606	52.838	62.238	57.002	1.00	25.15	A	O
ATOM	4692	N	ILE	607	54.059	64.129	57.001	1.00	26.84	A	N
ATOM	4693	CA	ILE	607	54.607	63.915	58.337	1.00	28.30	A	C
ATOM	4694	CB	ILE	607	55.639	65.002	58.702	1.00	28.21	A	C
ATOM	4695	CG2	ILE	607	56.165	64.778	60.116	1.00	26.82	A	C
ATOM	4696	CG1	ILE	607	56.789	64.977	57.694	1.00	29.86	A	C
ATOM	4697	CD1	ILE	607	57.796	66.086	57.881	1.00	28.34	A	C
ATOM	4698	C	ILE	607	53.470	63.963	59.355	1.00	29.50	A	C
ATOM	4699	O	ILE	607	53.359	63.093	60.226	1.00	27.80	A	O
ATOM	4700	N	GLU	608	52.619	64.978	59.239	1.00	30.32	A	N
ATOM	4701	CA	GLU	608	51.508	65.099	60.164	1.00	32.21	A	C
ATOM	4702	CB	GLU	608	50.705	66.379	59.919	1.00	33.05	A	C
ATOM	4703	CG	GLU	608	49.578	66.581	60.936	1.00	34.99	A	C

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(Continued)

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ATOM	4704	CD	GLU	608	50.054	66.482	62.389	1.00	38.42	A	C
ATOM	4705	OE1	GLU	608	49.197	66.454	63.302	1.00	37.67	A	O
ATOM	4706	OE2	GLU	608	51.285	66.435	62.625	1.00	40.64	A	O
ATOM	4707	C	GLU	608	50.606	63.891	60.012	1.00	32.76	A	C
ATOM	4708	O	GLU	608	49.889	63.527	60.947	1.00	33.47	A	O
ATOM	4709	N	ALA	609	50.643	63.270	58.836	1.00	31.32	A	N
ATOM	4710	CA	ALA	609	49.827	62.090	58.595	1.00	30.73	A	C
ATOM	4711	CB	ALA	609	49.883	61.682	57.123	1.00	28.50	A	C
ATOM	4712	C	ALA	609	50.355	60.968	59.472	1.00	30.16	A	C
ATOM	4713	O	ALA	609	49.583	60.274	60.139	1.00	31.03	A	O
ATOM	4714	N	ALA	610	51.674	60.803	59.479	1.00	29.26	A	N
ATOM	4715	CA	ALA	610	52.310	59.758	60.274	1.00	28.48	A	C
ATOM	4716	CB	ALA	610	53.826	59.818	60.114	1.00	27.67	A	C
ATOM	4717	C	ALA	610	51.930	59.886	61.743	1.00	27.62	A	C
ATOM	4718	O	ALA	610	51.556	58.904	62.379	1.00	28.43	A	O
ATOM	4719	N	ARG	611	52.025	61.094	62.282	1.00	26.94	A	N
ATOM	4720	CA	ARG	611	51.674	61.309	63.678	1.00	28.98	A	C
ATOM	4721	CB	ARG	611	51.812	62.787	64.042	1.00	28.96	A	C
ATOM	4722	CG	ARG	611	53.239	63.291	64.032	1.00	29.26	A	C
ATOM	4723	CD	ARG	611	53.281	64.799	64.187	1.00	29.92	A	C
ATOM	4724	NE	ARG	611	54.641	65.322	64.102	1.00	28.90	A	N
ATOM	4725	CZ	ARG	611	54.980	66.384	63.378	1.00	29.97	A	C
ATOM	4726	NH1	ARG	611	54.055	67.028	62.680	1.00	31.41	A	N
ATOM	4727	NH2	ARG	611	56.237	66.802	63.347	1.00	29.57	A	N
ATOM	4728	C	ARG	611	50.242	60.846	63.923	1.00	29.90	A	C
ATOM	4729	O	ARG	611	49.983	60.084	64.856	1.00	31.08	A	O
ATOM	4730	N	GLN	612	49.319	61.298	63.076	1.00	30.18	A	N
ATOM	4731	CA	GLN	612	47.916	60.922	63.195	1.00	30.42	A	C
ATOM	4732	CB	GLN	612	47.108	61.497	62.035	1.00	30.55	A	C
ATOM	4733	CG	GLN	612	47.112	63.001	61.964	1.00	33.70	A	C
ATOM	4734	CD	GLN	612	46.446	63.637	63.162	1.00	34.91	A	C
ATOM	4735	OE1	GLN	612	45.276	63.379	63.444	1.00	35.03	A	O
ATOM	4736	NE2	GLN	612	47.188	64.475	63.875	1.00	35.30	A	N
ATOM	4737	C	GLN	612	47.740	59.405	63.223	1.00	30.70	A	C
ATOM	4738	O	GLN	612	46.993	58.878	64.049	1.00	31.56	A	O
ATOM	4739	N	PHE	613	48.415	58.698	62.324	1.00	30.50	A	N
ATOM	4740	CA	PHE	613	48.291	57.248	62.301	1.00	32.33	A	C
ATOM	4741	CB	PHE	613	49.043	56.653	61.114	1.00	31.37	A	C
ATOM	4742	CG	PHE	613	48.537	57.126	59.787	1.00	30.49	A	C
ATOM	4743	CD1	PHE	613	47.167	57.171	59.529	1.00	30.03	A	C
ATOM	4744	CD2	PHE	613	49.423	57.523	58.793	1.00	28.11	A	C
ATOM	4745	CE1	PHE	613	46.687	57.604	58.300	1.00	29.96	A	C
ATOM	4746	CE2	PHE	613	48.954	57.959	57.559	1.00	28.75	A	C
ATOM	4747	CZ	PHE	613	47.585	58.001	57.309	1.00	28.70	A	C
ATOM	4748	C	PHE	613	48.835	56.679	63.597	1.00	34.28	A	C
ATOM	4749	O	PHE	613	48.327	55.677	64.107	1.00	34.47	A	O
ATOM	4750	N	SER	614	49.865	57.326	64.134	1.00	35.61	A	N
ATOM	4751	CA	SER	614	50.454	56.884	65.388	1.00	37.88	A	C
ATOM	4752	CB	SER	614	51.723	57.677	65.683	1.00	38.32	A	C

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(Continued)

## FIG. 4 - 98

ATOM	4753	OG	SER	614	52.686	57.477	64.663	1.00	38.53	A	O
ATOM	4754	C	SER	614	49.424	57.098	66.494	1.00	39.76	A	C
ATOM	4755	O	SER	614	49.283	56.276	67.398	1.00	41.47	A	O
ATOM	4756	N	LYS	615	48.694	58.204	66.413	1.00	40.51	A	N
ATOM	4757	CA	LYS	615	47.663	58.490	67.400	1.00	41.32	A	C
ATOM	4758	CB	LYS	615	47.047	59.870	67.155	1.00	42.73	A	C
ATOM	4759	CG	LYS	615	47.884	61.040	67.642	1.00	44.59	A	C
ATOM	4760	CD	LYS	615	47.064	62.330	67.631	1.00	46.18	A	C
ATOM	4761	CE	LYS	615	47.864	63.511	68.168	1.00	46.73	A	C
ATOM	4762	NZ	LYS	615	48.314	63.301	69.577	1.00	48.03	A	N
ATOM	4763	C	LYS	615	46.552	57.441	67.347	1.00	40.86	A	C
ATOM	4764	O	LYS	615	45.794	57.285	68.303	1.00	41.94	A	O
ATOM	4765	N	MET	616	46.456	56.724	66.230	1.00	39.78	A	N
ATOM	4766	CA	MET	616	45.418	55.712	66.065	1.00	37.88	A	C
ATOM	4767	CB	MET	616	45.246	55.374	64.578	1.00	37.42	A	C
ATOM	4768	CG	MET	616	44.673	56.532	63.768	1.00	35.95	A	C
ATOM	4769	SD	MET	616	44.195	56.101	62.079	1.00	35.73	A	S
ATOM	4770	CE	MET	616	43.946	57.730	61.385	1.00	34.06	A	C
ATOM	4771	C	MET	616	45.654	54.447	66.885	1.00	36.90	A	C
ATOM	4772	O	MET	616	44.908	53.473	66.772	1.00	37.22	A	O
ATOM	4773	N	GLY	617	46.706	54.469	67.698	1.00	35.15	A	N
ATOM	4774	CA	GLY	617	47.013	53.355	68.578	1.00	32.74	A	C
ATOM	4775	C	GLY	617	47.445	51.995	68.065	1.00	32.72	A	C
ATOM	4776	O	GLY	617	47.806	51.143	68.872	1.00	33.71	A	O
ATOM	4777	N	PHE	618	47.409	51.751	66.761	1.00	32.52	A	N
ATOM	4778	CA	PHE	618	47.841	50.447	66.262	1.00	31.36	A	C
ATOM	4779	CB	PHE	618	46.701	49.759	65.496	1.00	31.10	A	C
ATOM	4780	CG	PHE	618	46.047	50.624	64.457	1.00	31.61	A	C
ATOM	4781	CD1	PHE	618	46.743	51.025	63.322	1.00	31.30	A	C
ATOM	4782	CD2	PHE	618	44.724	51.027	64.607	1.00	30.93	A	C
ATOM	4783	CE1	PHE	618	46.129	51.815	62.349	1.00	31.53	A	C
ATOM	4784	CE2	PHE	618	44.104	51.814	63.642	1.00	30.94	A	C
ATOM	4785	CZ	PHE	618	44.808	52.209	62.509	1.00	29.86	A	C
ATOM	4786	C	PHE	618	49.109	50.521	65.404	1.00	30.95	A	C
ATOM	4787	O	PHE	618	49.303	49.735	64.477	1.00	30.95	A	O
ATOM	4788	N	VAL	619	49.982	51.465	65.732	1.00	30.23	A	N
ATOM	4789	CA	VAL	619	51.226	51.627	64.996	1.00	29.99	A	C
ATOM	4790	CB	VAL	619	51.226	52.928	64.147	1.00	29.39	A	C
ATOM	4791	CG1	VAL	619	52.632	53.200	63.617	1.00	28.74	A	C
ATOM	4792	CG2	VAL	619	50.248	52.804	62.994	1.00	26.48	A	C
ATOM	4793	C	VAL	619	52.425	51.673	65.931	1.00	29.66	A	C
ATOM	4794	O	VAL	619	52.400	52.342	66.962	1.00	30.05	A	O
ATOM	4795	N	ASP	620	53.475	50.954	65.561	1.00	29.84	A	N
ATOM	4796	CA	ASP	620	54.695	50.932	66.347	1.00	29.07	A	C
ATOM	4797	CB	ASP	620	55.563	49.748	65.924	1.00	27.94	A	C
ATOM	4798	CG	ASP	620	56.789	49.587	66.794	1.00	27.02	A	C
ATOM	4799	OD1	ASP	620	57.191	50.580	67.439	1.00	26.38	A	O
ATOM	4800	OD2	ASP	620	57.358	48.473	66.818	1.00	25.22	A	O
ATOM	4801	C	ASP	620	55.408	52.243	66.039	1.00	30.30	A	C

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## FIG. 4 - 99

(Continued)

ATOM	4802	O	ASP	620	56.009	52.398	64.979	1.00	29.95	A	O
ATOM	4803	N	ASN	621	55.330	53.196	66.958	1.00	33.01	A	N
ATOM	4804	CA	ASN	621	55.962	54.492	66.746	1.00	35.15	A	C
ATOM	4805	CB	ASN	621	55.761	55.376	67.975	1.00	38.29	A	C
ATOM	4806	CG	ASN	621	56.420	54.804	69.214	1.00	43.03	A	C
ATOM	4807	OD1	ASN	621	57.648	54.821	69.346	1.00	44.79	A	O
ATOM	4808	ND2	ASN	621	55.606	54.280	70.130	1.00	45.61	A	N
ATOM	4809	C	ASN	621	57.453	54.370	66.441	1.00	35.20	A	C
ATOM	4810	O	ASN	621	58.083	55.330	66.004	1.00	34.67	A	O
ATOM	4811	N	LYS	622	58.016	53.186	66.660	1.00	36.30	A	N
ATOM	4812	CA	LYS	622	59.439	52.977	66.418	1.00	35.70	A	C
ATOM	4813	CB	LYS	622	60.030	52.027	67.464	1.00	37.42	A	C
ATOM	4814	CG	LYS	622	60.148	52.611	68.866	1.00	39.14	A	C
ATOM	4815	CD	LYS	622	60.763	51.584	69.804	1.00	43.05	A	C
ATOM	4816	CE	LYS	622	60.839	52.077	71.240	1.00	45.27	A	C
ATOM	4817	NZ	LYS	622	61.516	51.077	72.123	1.00	45.73	A	N
ATOM	4818	C	LYS	622	59.762	52.445	65.036	1.00	34.38	A	C
ATOM	4819	O	LYS	622	60.896	52.572	64.571	1.00	35.67	A	O
ATOM	4820	N	ARG	623	58.783	51.846	64.374	1.00	31.86	A	N
ATOM	4821	CA	ARG	623	59.030	51.308	63.046	1.00	29.60	A	C
ATOM	4822	CB	ARG	623	58.821	49.791	63.058	1.00	29.94	A	C
ATOM	4823	CG	ARG	623	59.767	49.071	64.009	1.00	32.12	A	C
ATOM	4824	CD	ARG	623	59.117	47.832	64.614	1.00	33.42	A	C
ATOM	4825	NE	ARG	623	59.247	46.663	63.758	1.00	34.25	A	N
ATOM	4826	CZ	ARG	623	58.457	45.601	63.833	1.00	34.36	A	C
ATOM	4827	NH1	ARG	623	57.476	45.572	64.725	1.00	35.41	A	N
ATOM	4828	NH2	ARG	623	58.655	44.571	63.021	1.00	33.15	A	N
ATOM	4829	C	ARG	623	58.179	51.957	61.962	1.00	27.66	A	C
ATOM	4830	O	ARG	623	57.315	51.313	61.363	1.00	27.44	A	O
ATOM	4831	N	ILE	624	58.425	53.241	61.720	1.00	25.16	A	N
ATOM	4832	CA	ILE	624	57.708	53.977	60.685	1.00	24.70	A	C
ATOM	4833	CB	ILE	624	57.114	55.298	61.224	1.00	24.52	A	C
ATOM	4834	CG2	ILE	624	56.391	56.025	60.107	1.00	23.47	A	C
ATOM	4835	CG1	ILE	624	56.136	55.021	62.371	1.00	24.01	A	C
ATOM	4836	CD1	ILE	624	55.473	56.277	62.936	1.00	19.15	A	C
ATOM	4837	C	ILE	624	58.667	54.311	59.532	1.00	24.37	A	C
ATOM	4838	O	ILE	624	59.651	55.034	59.709	1.00	23.38	A	O
ATOM	4839	N	ALA	625	58.384	53.768	58.356	1.00	22.58	A	N
ATOM	4840	CA	ALA	625	59.213	54.014	57.189	1.00	21.00	A	C
ATOM	4841	CB	ALA	625	59.650	52.693	56.579	1.00	20.21	A	C
ATOM	4842	C	ALA	625	58.430	54.833	56.168	1.00	21.28	A	C
ATOM	4843	O	ALA	625	57.209	54.966	56.275	1.00	21.90	A	O
ATOM	4844	N	ILE	626	59.135	55.385	55.185	1.00	19.63	A	N
ATOM	4845	CA	ILE	626	58.502	56.178	54.137	1.00	18.63	A	C
ATOM	4846	CB	ILE	626	58.589	57.699	54.446	1.00	18.98	A	C
ATOM	4847	CG2	ILE	626	60.032	58.103	54.694	1.00	18.36	A	C
ATOM	4848	CG1	ILE	626	57.973	58.501	53.296	1.00	19.11	A	C
ATOM	4849	CD1	ILE	626	57.872	59.991	53.562	1.00	18.34	A	C
ATOM	4850	C	ILE	626	59.185	55.882	52.809	1.00	17.48	A	C

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(Continued)

## FIG. 4 - 100

ATOM	4851	O	ILE	626	60.380	55.619	52.776	1.00	17.10	A	O
ATOM	4852	N	TRP	627	58.425	55.893	51.719	1.00	17.62	A	N
ATOM	4853	CA	TRP	627	58.998	55.622	50.409	1.00	17.62	A	C
ATOM	4854	CB	TRP	627	59.190	54.118	50.206	1.00	16.80	A	C
ATOM	4855	CG	TRP	627	58.096	53.441	49.427	1.00	18.70	A	C
ATOM	4856	CD2	TRP	627	58.139	53.055	48.044	1.00	17.58	A	C
ATOM	4857	CE2	TRP	627	56.912	52.425	47.749	1.00	17.70	A	C
ATOM	4858	CE3	TRP	627	59.095	53.179	47.028	1.00	15.10	A	C
ATOM	4859	CD1	TRP	627	56.879	53.047	49.895	1.00	18.68	A	C
ATOM	4860	NE1	TRP	627	56.163	52.435	48.896	1.00	18.72	A	N
ATOM	4861	CZ2	TRP	627	56.617	51.916	46.480	1.00	16.42	A	C
ATOM	4862	CZ3	TRP	627	58.801	52.673	45.769	1.00	14.48	A	C
ATOM	4863	CH2	TRP	627	57.575	52.048	45.507	1.00	14.63	A	C
ATOM	4864	C	TRP	627	58.157	56.191	49.275	1.00	18.48	A	C
ATOM	4865	O	TRP	627	56.934	56.280	49.381	1.00	18.15	A	O
ATOM	4866	N	GLY	628	58.829	56.579	48.193	1.00	18.70	A	N
ATOM	4867	CA	GLY	628	58.140	57.146	47.049	1.00	18.30	A	C
ATOM	4868	C	GLY	628	58.986	57.163	45.787	1.00	18.36	A	C
ATOM	4869	O	GLY	628	60.212	57.065	45.833	1.00	19.07	A	O
ATOM	4870	N	TRP	629	58.312	57.300	44.654	1.00	17.25	A	N
ATOM	4871	CA	TRP	629	58.945	57.322	43.343	1.00	15.27	A	C
ATOM	4872	CB	TRP	629	58.306	56.214	42.494	1.00	10.48	A	C
ATOM	4873	CG	TRP	629	59.131	55.698	41.357	1.00	10.84	A	C
ATOM	4874	CD2	TRP	629	59.512	54.335	41.122	1.00	9.02	A	C
ATOM	4875	CE2	TRP	629	60.243	54.310	39.914	1.00	10.87	A	C
ATOM	4876	CE3	TRP	629	59.312	53.135	41.818	1.00	9.31	A	C
ATOM	4877	CD1	TRP	629	59.635	56.422	40.313	1.00	10.72	A	C
ATOM	4878	NE1	TRP	629	60.299	55.595	39.443	1.00	10.74	A	N
ATOM	4879	CZ2	TRP	629	60.779	53.126	39.379	1.00	12.40	A	C
ATOM	4880	CZ3	TRP	629	59.842	51.959	41.295	1.00	11.95	A	C
ATOM	4881	CH2	TRP	629	60.571	51.965	40.080	1.00	13.29	A	C
ATOM	4882	C	TRP	629	58.671	58.722	42.753	1.00	15.91	A	C
ATOM	4883	O	TRP	629	57.622	59.300	43.012	1.00	15.58	A	O
ATOM	4884	N	SER	630	59.612	59.269	41.983	1.00	16.99	A	N
ATOM	4885	CA	SER	630	59.453	60.603	41.383	1.00	16.78	A	C
ATOM	4886	CB	SER	630	58.258	60.644	40.421	1.00	18.65	A	C
ATOM	4887	OG	SER	630	58.531	59.987	39.198	1.00	22.38	A	O
ATOM	4888	C	SER	630	59.234	61.656	42.450	1.00	16.69	A	C
ATOM	4889	O	SER	630	60.076	61.856	43.321	1.00	17.90	A	O
ATOM	4890	N	TYR	631	58.093	62.335	42.368	1.00	17.21	A	N
ATOM	4891	CA	TYR	631	57.737	63.362	43.335	1.00	15.51	A	C
ATOM	4892	CB	TYR	631	56.380	63.969	42.981	1.00	17.16	A	C
ATOM	4893	CG	TYR	631	56.161	65.353	43.545	1.00	18.38	A	C
ATOM	4894	CD1	TYR	631	55.947	65.550	44.909	1.00	18.79	A	C
ATOM	4895	CE1	TYR	631	55.741	66.826	45.429	1.00	19.48	A	C
ATOM	4896	CD2	TYR	631	56.168	66.470	42.714	1.00	18.85	A	C
ATOM	4897	CE2	TYR	631	55.963	67.751	43.226	1.00	19.30	A	C
ATOM	4898	CZ	TYR	631	55.748	67.918	44.580	1.00	19.21	A	C
ATOM	4899	OH	TYR	631	55.520	69.173	45.084	1.00	20.71	A	O

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## FIG. 4 - 101

(Continued)

ATOM	4900	C	TYR	631	57.672	62.632	44.668	1.00	15.27	A	C
ATOM	4901	O	TYR	631	57.946	63.201	45.731	1.00	13.23	A	O
ATOM	4902	N	GLY	632	57.324	61.350	44.592	1.00	14.83	A	N
ATOM	4903	CA	GLY	632	57.266	60.529	45.783	1.00	15.04	A	C
ATOM	4904	C	GLY	632	58.653	60.477	46.394	1.00	14.53	A	C
ATOM	4905	O	GLY	632	58.816	60.652	47.596	1.00	13.85	A	O
ATOM	4906	N	GLY	633	59.655	60.246	45.551	1.00	15.63	A	N
ATOM	4907	CA	GLY	633	61.030	60.185	46.014	1.00	14.69	A	C
ATOM	4908	C	GLY	633	61.500	61.513	46.576	1.00	15.25	A	C
ATOM	4909	O	GLY	633	62.251	61.561	47.555	1.00	16.82	A	O
ATOM	4910	N	TYR	634	61.058	62.598	45.954	1.00	13.67	A	N
ATOM	4911	CA	TYR	634	61.418	63.940	46.398	1.00	13.29	A	C
ATOM	4912	CB	TYR	634	60.901	64.964	45.397	1.00	11.67	A	C
ATOM	4913	CG	TYR	634	60.914	66.382	45.904	1.00	12.54	A	C
ATOM	4914	CD1	TYR	634	62.112	67.069	46.072	1.00	13.46	A	C
ATOM	4915	CE1	TYR	634	62.125	68.398	46.484	1.00	13.37	A	C
ATOM	4916	CD2	TYR	634	59.723	67.057	46.173	1.00	11.38	A	C
ATOM	4917	CE2	TYR	634	59.727	68.383	46.586	1.00	11.86	A	C
ATOM	4918	CZ	TYR	634	60.933	69.049	46.734	1.00	12.83	A	C
ATOM	4919	OH	TYR	634	60.957	70.375	47.091	1.00	12.97	A	O
ATOM	4920	C	TYR	634	60.829	64.240	47.778	1.00	14.36	A	C
ATOM	4921	O	TYR	634	61.524	64.721	48.672	1.00	16.28	A	O
ATOM	4922	N	VAL	635	59.542	63.968	47.949	1.00	14.99	A	N
ATOM	4923	CA	VAL	635	58.899	64.218	49.231	1.00	15.44	A	C
ATOM	4924	CB	VAL	635	57.364	64.025	49.135	1.00	15.15	A	C
ATOM	4925	CG1	VAL	635	56.743	63.988	50.524	1.00	14.56	A	C
ATOM	4926	CG2	VAL	635	56.758	65.167	48.326	1.00	12.62	A	C
ATOM	4927	C	VAL	635	59.486	63.296	50.294	1.00	16.48	A	C
ATOM	4928	O	VAL	635	59.681	63.711	51.439	1.00	16.89	A	O
ATOM	4929	N	THR	636	59.779	62.054	49.917	1.00	16.16	A	N
ATOM	4930	CA	THR	636	60.368	61.098	50.855	1.00	18.40	A	C
ATOM	4931	CB	THR	636	60.701	59.746	50.175	1.00	18.30	A	C
ATOM	4932	OG1	THR	636	59.504	59.130	49.696	1.00	20.57	A	O
ATOM	4933	CG2	THR	636	61.362	58.807	51.157	1.00	20.48	A	C
ATOM	4934	C	THR	636	61.676	61.676	51.396	1.00	19.91	A	C
ATOM	4935	O	THR	636	61.914	61.696	52.609	1.00	19.58	A	O
ATOM	4936	N	SER	637	62.524	62.141	50.483	1.00	19.89	A	N
ATOM	4937	CA	SER	637	63.804	62.711	50.862	1.00	20.30	A	C
ATOM	4938	CB	SER	637	64.599	63.086	49.614	1.00	19.17	A	C
ATOM	4939	OG	SER	637	64.823	61.952	48.800	1.00	19.07	A	O
ATOM	4940	C	SER	637	63.615	63.938	51.749	1.00	21.61	A	C
ATOM	4941	O	SER	637	64.235	64.049	52.812	1.00	22.54	A	O
ATOM	4942	N	MET	638	62.760	64.855	51.309	1.00	21.06	A	N
ATOM	4943	CA	MET	638	62.490	66.074	52.066	1.00	21.87	A	C
ATOM	4944	CB	MET	638	61.417	66.895	51.354	1.00	20.36	A	C
ATOM	4945	CG	MET	638	61.876	67.465	50.032	1.00	21.23	A	C
ATOM	4946	SD	MET	638	63.069	68.787	50.261	1.00	21.33	A	S
ATOM	4947	CE	MET	638	62.006	70.229	50.125	1.00	19.31	A	C
ATOM	4948	C	MET	638	62.039	65.748	53.494	1.00	21.51	A	C

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(Continued)

## FIG. 4 - 102

ATOM	4949	O	MET	638	62.511	66.351	54.472	1.00	19.64	A	O
ATOM	4950	N	VAL	639	61.116	64.798	53.600	1.00	19.63	A	N
ATOM	4951	CA	VAL	639	60.611	64.372	54.891	1.00	20.04	A	C
ATOM	4952	CB	VAL	639	59.524	63.287	54.746	1.00	20.08	A	C
ATOM	4953	CG1	VAL	639	59.201	62.688	56.112	1.00	20.55	A	C
ATOM	4954	CG2	VAL	639	58.275	63.879	54.108	1.00	17.95	A	C
ATOM	4955	C	VAL	639	61.758	63.793	55.692	1.00	20.25	A	C
ATOM	4956	O	VAL	639	61.986	64.185	56.831	1.00	23.11	A	O
ATOM	4957	N	LEU	640	62.489	62.864	55.088	1.00	20.83	A	N
ATOM	4958	CA	LEU	640	63.608	62.225	55.765	1.00	22.08	A	C
ATOM	4959	CB	LEU	640	64.245	61.179	54.855	1.00	22.31	A	C
ATOM	4960	CG	LEU	640	63.400	59.939	54.570	1.00	21.31	A	C
ATOM	4961	CD1	LEU	640	64.143	59.041	53.611	1.00	22.16	A	C
ATOM	4962	CD2	LEU	640	63.105	59.205	55.863	1.00	22.25	A	C
ATOM	4963	C	LEU	640	64.675	63.212	56.239	1.00	23.38	A	C
ATOM	4964	O	LEU	640	65.416	62.922	57.182	1.00	22.99	A	O
ATOM	4965	N	GLY	641	64.745	64.374	55.592	1.00	23.16	A	N
ATOM	4966	CA	GLY	641	65.731	65.368	55.972	1.00	23.10	A	C
ATOM	4967	C	GLY	641	65.153	66.555	56.721	1.00	23.73	A	C
ATOM	4968	O	GLY	641	65.782	67.609	56.802	1.00	23.94	A	O
ATOM	4969	N	SER	642	63.958	66.393	57.278	1.00	22.74	A	N
ATOM	4970	CA	SER	642	63.318	67.484	58.002	1.00	20.76	A	C
ATOM	4971	CB	SER	642	61.798	67.370	57.883	1.00	19.77	A	C
ATOM	4972	OG	SER	642	61.319	66.213	58.546	1.00	17.97	A	O
ATOM	4973	C	SER	642	63.723	67.488	59.471	1.00	21.73	A	C
ATOM	4974	O	SER	642	63.656	68.519	60.140	1.00	21.40	A	O
ATOM	4975	N	GLY	643	64.136	66.327	59.967	1.00	22.24	A	N
ATOM	4976	CA	GLY	643	64.548	66.213	61.350	1.00	22.64	A	C
ATOM	4977	C	GLY	643	63.407	65.944	62.314	1.00	23.74	A	C
ATOM	4978	O	GLY	643	63.585	66.064	63.528	1.00	25.32	A	O
ATOM	4979	N	SER	644	62.244	65.573	61.786	1.00	23.53	A	N
ATOM	4980	CA	SER	644	61.067	65.301	62.616	1.00	23.38	A	C
ATOM	4981	CB	SER	644	59.850	64.995	61.742	1.00	24.79	A	C
ATOM	4982	OG	SER	644	59.898	63.666	61.247	1.00	24.45	A	O
ATOM	4983	C	SER	644	61.287	64.129	63.559	1.00	23.18	A	C
ATOM	4984	O	SER	644	60.565	63.961	64.536	1.00	24.28	A	O
ATOM	4985	N	GLY	645	62.278	63.307	63.258	1.00	23.27	A	N
ATOM	4986	CA	GLY	645	62.543	62.166	64.107	1.00	24.80	A	C
ATOM	4987	C	GLY	645	61.398	61.175	64.114	1.00	24.80	A	C
ATOM	4988	O	GLY	645	61.379	60.248	64.920	1.00	27.93	A	O
ATOM	4989	N	VAL	646	60.446	61.357	63.207	1.00	23.98	A	N
ATOM	4990	CA	VAL	646	59.289	60.474	63.121	1.00	22.32	A	C
ATOM	4991	CB	VAL	646	58.092	61.207	62.473	1.00	24.36	A	C
ATOM	4992	CG1	VAL	646	56.945	60.230	62.215	1.00	22.37	A	C
ATOM	4993	CG2	VAL	646	57.636	62.351	63.381	1.00	24.11	A	C
ATOM	4994	C	VAL	646	59.552	59.202	62.327	1.00	21.28	A	C
ATOM	4995	O	VAL	646	59.079	58.128	62.690	1.00	21.25	A	O
ATOM	4996	N	PHE	647	60.303	59.326	61.239	1.00	21.00	A	N
ATOM	4997	CA	PHE	647	60.593	58.182	60.380	1.00	18.33	A	C

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(Continued)

## FIG. 4 - 103

ATOM	4998	CB	PHE	647	60.497	58.615	58.924	1.00	15.79	A	C
ATOM	4999	CG	PHE	647	59.142	59.131	58.551	1.00	16.11	A	C
ATOM	5000	CD1	PHE	647	58.138	58.258	58.152	1.00	15.39	A	C
ATOM	5001	CD2	PHE	647	58.841	60.479	58.680	1.00	14.43	A	C
ATOM	5002	CE1	PHE	647	56.855	58.722	57.894	1.00	13.82	A	C
ATOM	5003	CE2	PHE	647	57.562	60.943	58.423	1.00	15.28	A	C
ATOM	5004	CZ	PHE	647	56.568	60.061	58.031	1.00	13.75	A	C
ATOM	5005	C	PHE	647	61.944	57.555	60.663	1.00	18.46	A	C
ATOM	5006	O	PHE	647	62.943	58.250	60.825	1.00	20.84	A	O
ATOM	5007	N	LYS	648	61.958	56.232	60.722	1.00	17.11	A	N
ATOM	5008	CA	LYS	648	63.165	55.480	60.996	1.00	19.06	A	C
ATOM	5009	CB	LYS	648	62.789	54.105	61.545	1.00	17.86	A	C
ATOM	5010	CG	LYS	648	63.961	53.242	61.955	1.00	17.94	A	C
ATOM	5011	CD	LYS	648	63.484	51.869	62.405	1.00	19.57	A	C
ATOM	5012	CE	LYS	648	64.594	51.083	63.095	1.00	19.22	A	C
ATOM	5013	NZ	LYS	648	65.757	50.894	62.204	1.00	20.59	A	N
ATOM	5014	C	LYS	648	64.025	55.314	59.747	1.00	21.47	A	C
ATOM	5015	O	LYS	648	65.251	55.379	59.815	1.00	23.13	A	O
ATOM	5016	N	CYS	649	63.376	55.094	58.610	1.00	22.38	A	N
ATOM	5017	CA	CYS	649	64.077	54.898	57.353	1.00	24.23	A	C
ATOM	5018	C	CYS	649	63.156	55.237	56.181	1.00	24.09	A	C
ATOM	5019	O	CYS	649	61.939	55.319	56.342	1.00	23.94	A	O
ATOM	5020	CB	CYS	649	64.527	53.447	57.237	1.00	27.68	A	C
ATOM	5021	SG	CYS	649	63.130	52.287	57.313	1.00	32.05	A	S
ATOM	5022	N	GLY	650	63.746	55.426	55.004	1.00	21.50	A	N
ATOM	5023	CA	GLY	650	62.961	55.757	53.834	1.00	21.04	A	C
ATOM	5024	C	GLY	650	63.649	55.384	52.535	1.00	21.13	A	C
ATOM	5025	O	GLY	650	64.874	55.333	52.474	1.00	21.62	A	O
ATOM	5026	N	ILE	651	62.857	55.124	51.499	1.00	19.35	A	N
ATOM	5027	CA	ILE	651	63.388	54.753	50.195	1.00	19.18	A	C
ATOM	5028	CB	ILE	651	62.896	53.352	49.758	1.00	19.03	A	C
ATOM	5029	CG2	ILE	651	63.601	52.933	48.481	1.00	17.31	A	C
ATOM	5030	CG1	ILE	651	63.173	52.326	50.853	1.00	19.60	A	C
ATOM	5031	CD1	ILE	651	62.827	50.901	50.456	1.00	18.48	A	C
ATOM	5032	C	ILE	651	62.953	55.749	49.120	1.00	19.53	A	C
ATOM	5033	O	ILE	651	61.758	56.015	48.949	1.00	19.77	A	O
ATOM	5034	N	ALA	652	63.925	56.292	48.393	1.00	18.34	A	N
ATOM	5035	CA	ALA	652	63.633	57.240	47.324	1.00	15.69	A	C
ATOM	5036	CB	ALA	652	64.323	58.574	47.594	1.00	14.05	A	C
ATOM	5037	C	ALA	652	64.107	56.662	45.996	1.00	14.98	A	C
ATOM	5038	O	ALA	652	65.288	56.367	45.827	1.00	14.12	A	O
ATOM	5039	N	VAL	653	63.175	56.487	45.064	1.00	14.68	A	N
ATOM	5040	CA	VAL	653	63.492	55.963	43.738	1.00	14.84	A	C
ATOM	5041	CB	VAL	653	62.582	54.754	43.366	1.00	17.41	A	C
ATOM	5042	CG1	VAL	653	62.865	54.291	41.932	1.00	14.95	A	C
ATOM	5043	CG2	VAL	653	62.806	53.607	44.352	1.00	18.10	A	C
ATOM	5044	C	VAL	653	63.292	57.063	42.694	1.00	13.22	A	C
ATOM	5045	O	VAL	653	62.224	57.669	42.620	1.00	11.12	A	O
ATOM	5046	N	ALA	654	64.331	57.317	41.901	1.00	12.68	A	N

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## FIG. 4 - 104

(Continued)

ATOM	5047	CA	ALA	654	64.289	58.327	40.845	1.00	10.68	A	C
ATOM	5048	CB	ALA	654	63.513	57.790	39.650	1.00	7.27	A	C
ATOM	5049	C	ALA	654	63.653	59.607	41.352	1.00	10.02	A	C
ATOM	5050	O	ALA	654	62.687	60.103	40.787	1.00	13.18	A	O
ATOM	5051	N	PRO	655	64.208	60.179	42.420	1.00	10.68	A	N
ATOM	5052	CD	PRO	655	65.319	59.696	43.262	1.00	8.01	A	C
ATOM	5053	CA	PRO	655	63.643	61.408	42.971	1.00	10.40	A	C
ATOM	5054	CB	PRO	655	64.092	61.344	44.422	1.00	8.50	A	C
ATOM	5055	CG	PRO	655	65.476	60.822	44.277	1.00	6.23	A	C
ATOM	5056	C	PRO	655	64.090	62.714	42.327	1.00	12.92	A	C
ATOM	5057	O	PRO	655	65.166	62.793	41.717	1.00	13.38	A	O
ATOM	5058	N	VAL	656	63.245	63.735	42.454	1.00	12.39	A	N
ATOM	5059	CA	VAL	656	63.612	65.065	41.999	1.00	12.85	A	C
ATOM	5060	CB	VAL	656	62.373	65.946	41.769	1.00	11.42	A	C
ATOM	5061	CG1	VAL	656	62.781	67.416	41.645	1.00	10.52	A	C
ATOM	5062	CG2	VAL	656	61.661	65.500	40.510	1.00	10.18	A	C
ATOM	5063	C	VAL	656	64.382	65.560	43.236	1.00	13.79	A	C
ATOM	5064	O	VAL	656	64.038	65.188	44.355	1.00	14.63	A	O
ATOM	5065	N	SER	657	65.419	66.372	43.066	1.00	14.27	A	N
ATOM	5066	CA	SER	657	66.174	66.831	44.238	1.00	14.99	A	C
ATOM	5067	CB	SER	657	67.589	66.231	44.231	1.00	15.67	A	C
ATOM	5068	OG	SER	657	68.385	66.819	43.213	1.00	15.19	A	O
ATOM	5069	C	SER	657	66.286	68.343	44.320	1.00	14.77	A	C
ATOM	5070	O	SER	657	66.387	68.912	45.406	1.00	14.39	A	O
ATOM	5071	N	ARG	658	66.269	68.978	43.158	1.00	15.05	A	N
ATOM	5072	CA	ARG	658	66.388	70.423	43.038	1.00	16.33	A	C
ATOM	5073	CB	ARG	658	67.845	70.787	42.747	1.00	20.44	A	C
ATOM	5074	CG	ARG	658	68.142	72.274	42.582	1.00	24.34	A	C
ATOM	5075	CD	ARG	658	69.543	72.450	42.025	1.00	25.38	A	C
ATOM	5076	NE	ARG	658	69.905	73.838	41.757	1.00	25.70	A	N
ATOM	5077	CZ	ARG	658	70.353	74.683	42.676	1.00	28.34	A	C
ATOM	5078	NH1	ARG	658	70.491	74.288	43.935	1.00	28.23	A	N
ATOM	5079	NH2	ARG	658	70.690	75.916	42.329	1.00	29.55	A	N
ATOM	5080	C	ARG	658	65.515	70.775	41.850	1.00	15.87	A	C
ATOM	5081	O	ARG	658	65.752	70.288	40.735	1.00	16.75	A	O
ATOM	5082	N	TRP	659	64.514	71.616	42.073	1.00	13.52	A	N
ATOM	5083	CA	TRP	659	63.603	71.967	40.999	1.00	13.69	A	C
ATOM	5084	CB	TRP	659	62.465	72.823	41.550	1.00	13.63	A	C
ATOM	5085	CG	TRP	659	61.504	71.963	42.341	1.00	17.48	A	C
ATOM	5086	CD2	TRP	659	60.690	70.898	41.829	1.00	16.63	A	C
ATOM	5087	CE2	TRP	659	60.027	70.313	42.927	1.00	18.08	A	C
ATOM	5088	CE3	TRP	659	60.460	70.382	40.547	1.00	16.21	A	C
ATOM	5089	CD1	TRP	659	61.300	71.980	43.692	1.00	17.21	A	C
ATOM	5090	NE1	TRP	659	60.418	70.993	44.050	1.00	17.37	A	N
ATOM	5091	CZ2	TRP	659	59.145	69.233	42.785	1.00	21.55	A	C
ATOM	5092	CZ3	TRP	659	59.584	69.311	40.403	1.00	18.00	A	C
ATOM	5093	CH2	TRP	659	58.937	68.746	41.516	1.00	20.15	A	C
ATOM	5094	C	TRP	659	64.219	72.580	39.748	1.00	13.15	A	C
ATOM	5095	O	TRP	659	63.643	72.503	38.670	1.00	11.17	A	O

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## FIG. 4 - 105

(Continued)

ATOM	5096	N	GLU	660	65.400	73.163	39.871	1.00	14.12	A	N
ATOM	5097	CA	GLU	660	66.042	73.725	38.697	1.00	15.96	A	C
ATOM	5098	CB	GLU	660	67.147	74.704	39.108	1.00	16.83	A	C
ATOM	5099	CG	GLU	660	66.548	76.001	39.626	1.00	19.65	A	C
ATOM	5100	CD	GLU	660	67.535	76.901	40.313	1.00	22.71	A	C
ATOM	5101	OE1	GLU	660	68.310	77.600	39.617	1.00	25.18	A	O
ATOM	5102	OE2	GLU	660	67.527	76.907	41.561	1.00	23.59	A	O
ATOM	5103	C	GLU	660	66.577	72.635	37.777	1.00	15.29	A	C
ATOM	5104	O	GLU	660	67.001	72.922	36.659	1.00	16.67	A	O
ATOM	5105	N	TYR	661	66.539	71.383	38.233	1.00	14.54	A	N
ATOM	5106	CA	TYR	661	67.003	70.269	37.399	1.00	14.57	A	C
ATOM	5107	CB	TYR	661	67.642	69.154	38.230	1.00	13.59	A	C
ATOM	5108	CG	TYR	661	68.878	69.504	39.035	1.00	15.73	A	C
ATOM	5109	CD1	TYR	661	69.743	70.531	38.655	1.00	13.37	A	C
ATOM	5110	CE1	TYR	661	70.889	70.805	39.390	1.00	12.74	A	C
ATOM	5111	CD2	TYR	661	69.199	68.765	40.166	1.00	16.63	A	C
ATOM	5112	CE2	TYR	661	70.338	69.027	40.898	1.00	16.03	A	C
ATOM	5113	CZ	TYR	661	71.183	70.041	40.515	1.00	13.47	A	C
ATOM	5114	OH	TYR	661	72.322	70.252	41.267	1.00	8.43	A	O
ATOM	5115	C	TYR	661	65.842	69.637	36.608	1.00	15.74	A	C
ATOM	5116	O	TYR	661	66.077	68.854	35.675	1.00	13.97	A	O
ATOM	5117	N	TYR	662	64.602	69.963	36.984	1.00	13.28	A	N
ATOM	5118	CA	TYR	662	63.445	69.390	36.308	1.00	13.00	A	C
ATOM	5119	CB	TYR	662	62.305	69.143	37.308	1.00	14.01	A	C
ATOM	5120	CG	TYR	662	61.395	68.026	36.862	1.00	14.50	A	C
ATOM	5121	CD1	TYR	662	60.010	68.199	36.802	1.00	15.74	A	C
ATOM	5122	CE1	TYR	662	59.184	67.201	36.273	1.00	14.99	A	C
ATOM	5123	CD2	TYR	662	61.930	66.825	36.400	1.00	14.83	A	C
ATOM	5124	CE2	TYR	662	61.122	65.830	35.873	1.00	15.13	A	C
ATOM	5125	CZ	TYR	662	59.756	66.024	35.804	1.00	15.11	A	C
ATOM	5126	OH	TYR	662	58.983	65.060	35.214	1.00	17.05	A	O
ATOM	5127	C	TYR	662	62.964	70.251	35.135	1.00	12.46	A	C
ATOM	5128	O	TYR	662	63.320	71.423	35.030	1.00	12.22	A	O
ATOM	5129	N	ASP	663	62.147	69.673	34.260	1.00	12.09	A	N
ATOM	5130	CA	ASP	663	61.686	70.394	33.076	1.00	13.20	A	C
ATOM	5131	CB	ASP	663	60.998	69.427	32.099	1.00	11.88	A	C
ATOM	5132	CG	ASP	663	59.668	68.925	32.606	1.00	13.51	A	C
ATOM	5133	OD1	ASP	663	59.476	67.692	32.633	1.00	14.06	A	O
ATOM	5134	OD2	ASP	663	58.809	69.758	32.962	1.00	11.87	A	O
ATOM	5135	C	ASP	663	60.807	71.625	33.300	1.00	13.03	A	C
ATOM	5136	O	ASP	663	60.036	71.713	34.260	1.00	12.71	A	O
ATOM	5137	N	SER	664	60.945	72.576	32.383	1.00	12.83	A	N
ATOM	5138	CA	SER	664	60.210	73.829	32.425	1.00	13.80	A	C
ATOM	5139	CB	SER	664	60.433	74.600	31.120	1.00	14.92	A	C
ATOM	5140	OG	SER	664	59.996	73.851	30.000	1.00	14.78	A	O
ATOM	5141	C	SER	664	58.715	73.688	32.674	1.00	13.35	A	C
ATOM	5142	O	SER	664	58.234	73.974	33.762	1.00	15.82	A	O
ATOM	5143	N	VAL	665	57.987	73.247	31.658	1.00	13.43	A	N
ATOM	5144	CA	VAL	665	56.540	73.101	31.733	1.00	14.34	A	C

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## FIG. 4 - 106

(Continued)

ATOM	5145	CB	VAL	665	56.027	72.182	30.602	1.00	14.98	A	C
ATOM	5146	CG1	VAL	665	54.496	72.131	30.615	1.00	15.10	A	C
ATOM	5147	CG2	VAL	665	56.537	72.690	29.263	1.00	13.19	A	C
ATOM	5148	C	VAL	665	55.972	72.620	33.070	1.00	14.50	A	C
ATOM	5149	O	VAL	665	55.153	73.302	33.677	1.00	14.33	A	O
ATOM	5150	N	TYR	666	56.392	71.452	33.534	1.00	15.45	A	N
ATOM	5151	CA	TYR	666	55.876	70.948	34.801	1.00	17.06	A	C
ATOM	5152	CB	TYR	666	56.323	69.501	35.038	1.00	15.58	A	C
ATOM	5153	CG	TYR	666	55.839	68.903	36.349	1.00	13.94	A	C
ATOM	5154	CD1	TYR	666	54.692	68.119	36.395	1.00	14.70	A	C
ATOM	5155	CE1	TYR	666	54.276	67.517	37.577	1.00	13.28	A	C
ATOM	5156	CD2	TYR	666	56.560	69.080	37.534	1.00	13.77	A	C
ATOM	5157	CE2	TYR	666	56.154	68.482	38.727	1.00	12.27	A	C
ATOM	5158	CZ	TYR	666	55.012	67.700	38.737	1.00	15.52	A	C
ATOM	5159	OH	TYR	666	54.609	67.072	39.896	1.00	18.37	A	O
ATOM	5160	C	TYR	666	56.297	71.796	35.998	1.00	17.89	A	C
ATOM	5161	O	TYR	666	55.451	72.200	36.795	1.00	19.29	A	O
ATOM	5162	N	THR	667	57.592	72.066	36.125	1.00	17.90	A	N
ATOM	5163	CA	THR	667	58.092	72.833	37.265	1.00	19.74	A	C
ATOM	5164	CB	THR	667	59.621	72.953	37.251	1.00	18.84	A	C
ATOM	5165	OG1	THR	667	60.206	71.675	36.968	1.00	20.18	A	O
ATOM	5166	CG2	THR	667	60.108	73.441	38.604	1.00	17.74	A	C
ATOM	5167	C	THR	667	57.537	74.246	37.339	1.00	21.44	A	C
ATOM	5168	O	THR	667	56.916	74.635	38.333	1.00	21.51	A	O
ATOM	5169	N	GLU	668	57.778	75.011	36.280	1.00	21.85	A	N
ATOM	5170	CA	GLU	668	57.330	76.389	36.200	1.00	21.18	A	C
ATOM	5171	CB	GLU	668	57.746	76.976	34.859	1.00	20.69	A	C
ATOM	5172	CG	GLU	668	59.251	77.096	34.703	1.00	20.20	A	C
ATOM	5173	CD	GLU	668	59.657	77.559	33.322	1.00	19.55	A	C
ATOM	5174	OE1	GLU	668	58.783	78.068	32.588	1.00	19.49	A	O
ATOM	5175	OE2	GLU	668	60.851	77.422	32.977	1.00	18.34	A	O
ATOM	5176	C	GLU	668	55.828	76.517	36.394	1.00	21.50	A	C
ATOM	5177	O	GLU	668	55.339	77.559	36.814	1.00	22.31	A	O
ATOM	5178	N	ARG	669	55.098	75.449	36.101	1.00	21.90	A	N
ATOM	5179	CA	ARG	669	53.648	75.458	36.249	1.00	21.18	A	C
ATOM	5180	CB	ARG	669	53.060	74.121	35.786	1.00	22.06	A	C
ATOM	5181	CG	ARG	669	51.546	74.026	35.922	1.00	21.37	A	C
ATOM	5182	CD	ARG	669	51.085	72.625	35.653	1.00	20.85	A	C
ATOM	5183	NE	ARG	669	51.467	72.187	34.319	1.00	21.84	A	N
ATOM	5184	CZ	ARG	669	51.667	70.918	33.981	1.00	21.10	A	C
ATOM	5185	NH1	ARG	669	51.522	69.962	34.888	1.00	19.62	A	N
ATOM	5186	NH2	ARG	669	52.018	70.610	32.741	1.00	20.23	A	N
ATOM	5187	C	ARG	669	53.246	75.706	37.695	1.00	21.23	A	C
ATOM	5188	O	ARG	669	52.209	76.306	37.957	1.00	20.45	A	O
ATOM	5189	N	TYR	670	54.067	75.239	38.631	1.00	21.65	A	N
ATOM	5190	CA	TYR	670	53.771	75.409	40.047	1.00	22.27	A	C
ATOM	5191	CB	TYR	670	53.752	74.048	40.764	1.00	21.10	A	C
ATOM	5192	CG	TYR	670	53.113	72.930	39.972	1.00	20.47	A	C
ATOM	5193	CD1	TYR	670	53.896	71.995	39.310	1.00	20.74	A	C

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(Continued)

## FIG. 4 - 107

ATOM	5194	CE1	TYR	670	53.321	70.985	38.537	1.00	22.18	A	C
ATOM	5195	CD2	TYR	670	51.726	72.831	39.850	1.00	19.78	A	C
ATOM	5196	CE2	TYR	670	51.139	71.831	39.079	1.00	19.87	A	C
ATOM	5197	CZ	TYR	670	51.944	70.911	38.422	1.00	22.17	A	C
ATOM	5198	OH	TYR	670	51.388	69.931	37.623	1.00	23.11	A	O
ATOM	5199	C	TYR	670	54.769	76.317	40.757	1.00	23.32	A	C
ATOM	5200	O	TYR	670	54.442	76.937	41.763	1.00	24.86	A	O
ATOM	5201	N	MET	671	55.983	76.404	40.228	1.00	24.66	A	N
ATOM	5202	CA	MET	671	57.029	77.207	40.851	1.00	23.96	A	C
ATOM	5203	CB	MET	671	58.327	76.400	40.905	1.00	24.00	A	C
ATOM	5204	CG	MET	671	58.288	75.215	41.852	1.00	23.55	A	C
ATOM	5205	SD	MET	671	58.383	75.732	43.565	1.00	24.97	A	S
ATOM	5206	CE	MET	671	60.159	75.998	43.721	1.00	21.94	A	C
ATOM	5207	C	MET	671	57.330	78.547	40.203	1.00	24.00	A	C
ATOM	5208	O	MET	671	58.101	79.331	40.756	1.00	25.98	A	O
ATOM	5209	N	GLY	672	56.741	78.822	39.045	1.00	22.07	A	N
ATOM	5210	CA	GLY	672	57.044	80.076	38.379	1.00	22.40	A	C
ATOM	5211	C	GLY	672	58.472	80.028	37.857	1.00	22.69	A	C
ATOM	5212	O	GLY	672	59.005	78.947	37.641	1.00	23.27	A	O
ATOM	5213	N	LEU	673	59.108	81.180	37.667	1.00	22.65	A	N
ATOM	5214	CA	LEU	673	60.477	81.209	37.151	1.00	20.90	A	C
ATOM	5215	CB	LEU	673	60.626	82.356	36.164	1.00	19.50	A	C
ATOM	5216	CG	LEU	673	59.639	82.282	35.010	1.00	19.96	A	C
ATOM	5217	CD1	LEU	673	59.779	83.513	34.147	1.00	20.87	A	C
ATOM	5218	CD2	LEU	673	59.892	81.027	34.203	1.00	21.63	A	C
ATOM	5219	C	LEU	673	61.528	81.344	38.248	1.00	21.08	A	C
ATOM	5220	O	LEU	673	61.313	82.028	39.239	1.00	21.87	A	O
ATOM	5221	N	PRO	674	62.692	80.700	38.072	1.00	21.90	A	N
ATOM	5222	CD	PRO	674	63.050	79.803	36.968	1.00	21.16	A	C
ATOM	5223	CA	PRO	674	63.780	80.747	39.050	1.00	23.23	A	C
ATOM	5224	CB	PRO	674	64.618	79.510	38.709	1.00	21.90	A	C
ATOM	5225	CG	PRO	674	63.803	78.755	37.695	1.00	22.34	A	C
ATOM	5226	C	PRO	674	64.617	82.023	38.943	1.00	24.90	A	C
ATOM	5227	O	PRO	674	65.841	81.977	39.028	1.00	26.10	A	O
ATOM	5228	N	THR	675	63.966	83.158	38.743	1.00	25.88	A	N
ATOM	5229	CA	THR	675	64.695	84.411	38.640	1.00	27.60	A	C
ATOM	5230	CB	THR	675	64.208	85.237	37.447	1.00	27.12	A	C
ATOM	5231	OG1	THR	675	62.811	85.524	37.599	1.00	29.30	A	O
ATOM	5232	CG2	THR	675	64.431	84.471	36.156	1.00	25.59	A	C
ATOM	5233	C	THR	675	64.496	85.211	39.918	1.00	28.74	A	C
ATOM	5234	O	THR	675	63.543	84.982	40.660	1.00	29.47	A	O
ATOM	5235	N	PRO	676	65.404	86.156	40.200	1.00	29.41	A	N
ATOM	5236	CD	PRO	676	66.625	86.508	39.457	1.00	28.96	A	C
ATOM	5237	CA	PRO	676	65.284	86.969	41.411	1.00	29.70	A	C
ATOM	5238	CB	PRO	676	66.465	87.929	41.299	1.00	28.87	A	C
ATOM	5239	CG	PRO	676	67.467	87.142	40.533	1.00	28.27	A	C
ATOM	5240	C	PRO	676	63.948	87.707	41.484	1.00	30.03	A	C
ATOM	5241	O	PRO	676	63.359	87.829	42.558	1.00	29.93	A	O
ATOM	5242	N	GLU	677	63.463	88.190	40.343	1.00	30.62	A	N

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(Continued)

## FIG. 4 - 108

ATOM	5243	CA	GLU	677	62.203	88.923	40.348	1.00	30.92	A	C
ATOM	5244	CB	GLU	677	62.192	90.013	39.264	1.00	32.38	A	C
ATOM	5245	CG	GLU	677	62.103	89.536	37.821	1.00	34.78	A	C
ATOM	5246	CD	GLU	677	63.380	88.877	37.331	1.00	37.04	A	C
ATOM	5247	OE1	GLU	677	64.480	89.356	37.697	1.00	35.11	A	O
ATOM	5248	OE2	GLU	677	63.276	87.891	36.566	1.00	37.80	A	O
ATOM	5249	C	GLU	677	60.952	88.065	40.231	1.00	30.10	A	C
ATOM	5250	O	GLU	677	59.893	88.564	39.849	1.00	31.67	A	O
ATOM	5251	N	ASP	678	61.067	86.777	40.546	1.00	28.40	A	N
ATOM	5252	CA	ASP	678	59.906	85.897	40.523	1.00	26.09	A	C
ATOM	5253	CB	ASP	678	59.833	85.048	39.253	1.00	25.88	A	C
ATOM	5254	CG	ASP	678	58.472	84.359	39.097	1.00	28.22	A	C
ATOM	5255	OD1	ASP	678	57.885	83.980	40.128	1.00	28.64	A	O
ATOM	5256	OD2	ASP	678	57.980	84.189	37.956	1.00	28.80	A	O
ATOM	5257	C	ASP	678	59.920	84.982	41.737	1.00	25.86	A	C
ATOM	5258	O	ASP	678	59.481	85.382	42.810	1.00	28.55	A	O
ATOM	5259	N	ASN	679	60.442	83.768	41.591	1.00	23.97	A	N
ATOM	5260	CA	ASN	679	60.443	82.835	42.708	1.00	21.47	A	C
ATOM	5261	CB	ASN	679	59.326	81.818	42.496	1.00	19.41	A	C
ATOM	5262	CG	ASN	679	58.894	81.146	43.778	1.00	19.58	A	C
ATOM	5263	OD1	ASN	679	58.491	79.981	43.775	1.00	20.44	A	O
ATOM	5264	ND2	ASN	679	58.957	81.879	44.882	1.00	18.70	A	N
ATOM	5265	C	ASN	679	61.760	82.099	42.957	1.00	21.79	A	C
ATOM	5266	O	ASN	679	61.770	81.055	43.601	1.00	21.89	A	O
ATOM	5267	N	LEU	680	62.873	82.636	42.472	1.00	24.38	A	N
ATOM	5268	CA	LEU	680	64.164	81.967	42.665	1.00	26.33	A	C
ATOM	5269	CB	LEU	680	65.316	82.842	42.157	1.00	26.74	A	C
ATOM	5270	CG	LEU	680	66.726	82.275	42.385	1.00	28.22	A	C
ATOM	5271	CD1	LEU	680	66.844	80.903	41.747	1.00	30.03	A	C
ATOM	5272	CD2	LEU	680	67.772	83.211	41.801	1.00	29.33	A	C
ATOM	5273	C	LEU	680	64.449	81.556	44.109	1.00	27.18	A	C
ATOM	5274	O	LEU	680	64.977	80.471	44.347	1.00	28.31	A	O
ATOM	5275	N	ASP	681	64.111	82.411	45.072	1.00	27.79	A	N
ATOM	5276	CA	ASP	681	64.360	82.091	46.475	1.00	28.03	A	C
ATOM	5277	CB	ASP	681	63.836	83.196	47.394	1.00	30.36	A	C
ATOM	5278	CG	ASP	681	64.774	84.386	47.473	1.00	34.23	A	C
ATOM	5279	OD1	ASP	681	65.908	84.289	46.952	1.00	35.59	A	O
ATOM	5280	OD2	ASP	681	64.380	85.417	48.067	1.00	36.71	A	O
ATOM	5281	C	ASP	681	63.773	80.753	46.920	1.00	27.55	A	C
ATOM	5282	O	ASP	681	64.428	80.005	47.647	1.00	28.05	A	O
ATOM	5283	N	HIS	682	62.551	80.438	46.502	1.00	25.37	A	N
ATOM	5284	CA	HIS	682	61.981	79.164	46.913	1.00	25.07	A	C
ATOM	5285	CB	HIS	682	60.456	79.161	46.801	1.00	25.14	A	C
ATOM	5286	CG	HIS	682	59.832	77.914	47.349	1.00	27.18	A	C
ATOM	5287	CD2	HIS	682	59.091	76.948	46.754	1.00	27.87	A	C
ATOM	5288	ND1	HIS	682	60.021	77.503	48.650	1.00	26.29	A	N
ATOM	5289	CE1	HIS	682	59.428	76.336	48.832	1.00	26.61	A	C
ATOM	5290	NE2	HIS	682	58.857	75.977	47.697	1.00	25.03	A	N
ATOM	5291	C	HIS	682	62.559	77.983	46.130	1.00	24.30	A	C

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(Continued)

## FIG. 4 - 109

ATOM	5292	O	HIS	682	62.463	76.837	46.572	1.00	23.47	A	O
ATOM	5293	N	TYR	683	63.144	78.258	44.966	1.00	23.49	A	N
ATOM	5294	CA	TYR	683	63.768	77.208	44.157	1.00	22.64	A	C
ATOM	5295	CB	TYR	683	64.249	77.758	42.812	1.00	20.68	A	C
ATOM	5296	CG	TYR	683	63.291	77.594	41.655	1.00	19.28	A	C
ATOM	5297	CD1	TYR	683	63.325	76.461	40.857	1.00	16.29	A	C
ATOM	5298	CE1	TYR	683	62.464	76.317	39.783	1.00	16.83	A	C
ATOM	5299	CD2	TYR	683	62.361	78.589	41.347	1.00	20.47	A	C
ATOM	5300	CE2	TYR	683	61.495	78.453	40.276	1.00	20.17	A	C
ATOM	5301	CZ	TYR	683	61.554	77.314	39.500	1.00	19.09	A	C
ATOM	5302	OH	TYR	683	60.695	77.176	38.441	1.00	21.54	A	O
ATOM	5303	C	TYR	683	64.989	76.727	44.924	1.00	22.32	A	C
ATOM	5304	O	TYR	683	65.189	75.533	45.125	1.00	22.65	A	O
ATOM	5305	N	ARG	684	65.799	77.685	45.355	1.00	22.44	A	N
ATOM	5306	CA	ARG	684	67.025	77.392	46.076	1.00	22.97	A	C
ATOM	5307	CB	ARG	684	67.928	78.624	46.071	1.00	22.89	A	C
ATOM	5308	CG	ARG	684	68.349	79.064	44.672	1.00	24.57	A	C
ATOM	5309	CD	ARG	684	69.238	78.020	44.004	1.00	23.11	A	C
ATOM	5310	NE	ARG	684	69.328	78.223	42.562	1.00	25.47	A	N
ATOM	5311	CZ	ARG	684	69.844	79.299	41.974	1.00	27.89	A	C
ATOM	5312	NH1	ARG	684	70.337	80.294	42.703	1.00	29.09	A	N
ATOM	5313	NH2	ARG	684	69.846	79.388	40.648	1.00	27.04	A	N
ATOM	5314	C	ARG	684	66.807	76.922	47.501	1.00	22.90	A	C
ATOM	5315	O	ARG	684	67.711	76.368	48.111	1.00	24.16	A	O
ATOM	5316	N	ASN	685	65.608	77.121	48.030	1.00	24.64	A	N
ATOM	5317	CA	ASN	685	65.331	76.715	49.399	1.00	24.41	A	C
ATOM	5318	CB	ASN	685	64.599	77.831	50.134	1.00	28.42	A	C
ATOM	5319	CG	ASN	685	64.455	77.547	51.610	1.00	34.24	A	C
ATOM	5320	OD1	ASN	685	65.410	77.117	52.266	1.00	38.25	A	O
ATOM	5321	ND2	ASN	685	63.264	77.791	52.150	1.00	37.49	A	N
ATOM	5322	C	ASN	685	64.545	75.419	49.537	1.00	23.72	A	C
ATOM	5323	O	ASN	685	64.356	74.929	50.649	1.00	23.86	A	O
ATOM	5324	N	SER	686	64.101	74.852	48.417	1.00	21.55	A	N
ATOM	5325	CA	SER	686	63.336	73.613	48.457	1.00	19.71	A	C
ATOM	5326	CB	SER	686	61.976	73.811	47.774	1.00	19.20	A	C
ATOM	5327	OG	SER	686	62.114	74.112	46.397	1.00	15.00	A	O
ATOM	5328	C	SER	686	64.060	72.421	47.823	1.00	20.13	A	C
ATOM	5329	O	SER	686	63.447	71.611	47.128	1.00	21.27	A	O
ATOM	5330	N	THR	687	65.362	72.307	48.060	1.00	19.02	A	N
ATOM	5331	CA	THR	687	66.122	71.189	47.509	1.00	17.15	A	C
ATOM	5332	CB	THR	687	67.441	71.665	46.906	1.00	16.10	A	C
ATOM	5333	OG1	THR	687	68.362	71.959	47.960	1.00	17.42	A	O
ATOM	5334	CG2	THR	687	67.214	72.920	46.058	1.00	14.71	A	C
ATOM	5335	C	THR	687	66.433	70.153	48.585	1.00	15.79	A	C
ATOM	5336	O	THR	687	66.496	70.466	49.763	1.00	15.82	A	O
ATOM	5337	N	VAL	688	66.627	68.908	48.182	1.00	18.43	A	N
ATOM	5338	CA	VAL	688	66.935	67.854	49.147	1.00	17.92	A	C
ATOM	5339	CB	VAL	688	66.840	66.453	48.480	1.00	17.13	A	C
ATOM	5340	CG1	VAL	688	67.092	65.352	49.503	1.00	15.01	A	C

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## FIG. 4 - 110

(Continued)

ATOM	5341	CG2	VAL	688	65.459	66.279	47.845	1.00	18.49	A	C
ATOM	5342	C	VAL	688	68.341	68.059	49.720	1.00	17.50	A	C
ATOM	5343	O	VAL	688	68.559	67.905	50.923	1.00	15.69	A	O
ATOM	5344	N	MET	689	69.280	68.428	48.851	1.00	16.92	A	N
ATOM	5345	CA	MET	689	70.672	68.647	49.246	1.00	17.40	A	C
ATOM	5346	CB	MET	689	71.475	69.213	48.065	1.00	13.91	A	C
ATOM	5347	CG	MET	689	71.829	68.210	46.984	1.00	10.55	A	C
ATOM	5348	SD	MET	689	70.465	67.740	45.909	1.00	11.73	A	S
ATOM	5349	CE	MET	689	70.338	69.210	44.871	1.00	9.36	A	C
ATOM	5350	C	MET	689	70.897	69.539	50.479	1.00	17.90	A	C
ATOM	5351	O	MET	689	71.721	69.220	51.341	1.00	16.90	A	O
ATOM	5352	N	SER	690	70.179	70.653	50.569	1.00	18.32	A	N
ATOM	5353	CA	SER	690	70.358	71.544	51.712	1.00	21.65	A	C
ATOM	5354	CB	SER	690	69.621	72.866	51.501	1.00	20.29	A	C
ATOM	5355	OG	SER	690	68.234	72.702	51.711	1.00	24.78	A	O
ATOM	5356	C	SER	690	69.898	70.933	53.038	1.00	22.31	A	C
ATOM	5357	O	SER	690	69.930	71.606	54.063	1.00	23.43	A	O
ATOM	5358	N	ARG	691	69.480	69.672	53.023	1.00	21.70	A	N
ATOM	5359	CA	ARG	691	69.041	69.012	54.249	1.00	23.07	A	C
ATOM	5360	CB	ARG	691	67.591	68.546	54.113	1.00	22.90	A	C
ATOM	5361	CG	ARG	691	66.623	69.652	53.770	1.00	22.81	A	C
ATOM	5362	CD	ARG	691	65.201	69.152	53.813	1.00	22.97	A	C
ATOM	5363	NE	ARG	691	64.236	70.240	53.694	1.00	24.03	A	N
ATOM	5364	CZ	ARG	691	62.963	70.134	54.061	1.00	26.18	A	C
ATOM	5365	NH1	ARG	691	62.509	68.989	54.566	1.00	25.20	A	N
ATOM	5366	NH2	ARG	691	62.149	71.172	53.946	1.00	26.01	A	N
ATOM	5367	C	ARG	691	69.922	67.811	54.593	1.00	24.24	A	C
ATOM	5368	O	ARG	691	69.595	67.031	55.488	1.00	25.28	A	O
ATOM	5369	N	ALA	692	71.041	67.675	53.889	1.00	24.03	A	N
ATOM	5370	CA	ALA	692	71.960	66.561	54.100	1.00	24.84	A	C
ATOM	5371	CB	ALA	692	73.270	66.826	53.360	1.00	24.20	A	C
ATOM	5372	C	ALA	692	72.251	66.210	55.562	1.00	24.60	A	C
ATOM	5373	O	ALA	692	72.066	65.068	55.967	1.00	24.83	A	O
ATOM	5374	N	GLU	693	72.707	67.181	56.347	1.00	25.74	A	N
ATOM	5375	CA	GLU	693	73.033	66.944	57.757	1.00	27.13	A	C
ATOM	5376	CB	GLU	693	73.351	68.266	58.463	1.00	29.38	A	C
ATOM	5377	CG	GLU	693	74.829	68.606	58.583	1.00	35.02	A	C
ATOM	5378	CD	GLU	693	75.604	67.627	59.463	1.00	39.06	A	C
ATOM	5379	OE1	GLU	693	74.984	66.948	60.316	1.00	38.42	A	O
ATOM	5380	OE2	GLU	693	76.845	67.554	59.307	1.00	41.03	A	O
ATOM	5381	C	GLU	693	71.947	66.215	58.549	1.00	26.16	A	C
ATOM	5382	O	GLU	693	72.250	65.505	59.506	1.00	26.78	A	O
ATOM	5383	N	ASN	694	70.688	66.387	58.160	1.00	24.46	A	N
ATOM	5384	CA	ASN	694	69.594	65.734	58.873	1.00	24.35	A	C
ATOM	5385	CB	ASN	694	68.274	66.473	58.619	1.00	26.79	A	C
ATOM	5386	CG	ASN	694	68.191	67.796	59.370	1.00	28.23	A	C
ATOM	5387	OD1	ASN	694	67.291	68.607	59.132	1.00	29.60	A	O
ATOM	5388	ND2	ASN	694	69.127	68.015	60.287	1.00	27.09	A	N
ATOM	5389	C	ASN	694	69.412	64.252	58.567	1.00	22.78	A	C

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(Continued)

## FIG. 4 - 1 1 1

ATOM	5390	O	ASN	694	68.736	63.555	59.318	1.00	22.09	A	O
ATOM	5391	N	PHE	695	70.008	63.764	57.481	1.00	21.23	A	N
ATOM	5392	CA	PHE	695	69.876	62.351	57.135	1.00	20.87	A	C
ATOM	5393	CB	PHE	695	70.297	62.085	55.686	1.00	18.97	A	C
ATOM	5394	CG	PHE	695	69.262	62.465	54.663	1.00	15.41	A	C
ATOM	5395	CD1	PHE	695	68.980	63.804	54.394	1.00	16.20	A	C
ATOM	5396	CD2	PHE	695	68.582	61.480	53.948	1.00	13.85	A	C
ATOM	5397	CE1	PHE	695	68.033	64.160	53.419	1.00	15.80	A	C
ATOM	5398	CE2	PHE	695	67.636	61.819	52.976	1.00	14.69	A	C
ATOM	5399	CZ	PHE	695	67.360	63.165	52.710	1.00	14.36	A	C
ATOM	5400	C	PHE	695	70.704	61.478	58.068	1.00	22.60	A	C
ATOM	5401	O	PHE	695	70.734	60.253	57.932	1.00	22.75	A	O
ATOM	5402	N	LYS	696	71.388	62.111	59.014	1.00	23.86	A	N
ATOM	5403	CA	LYS	696	72.189	61.369	59.980	1.00	24.30	A	C
ATOM	5404	CB	LYS	696	73.119	62.315	60.744	1.00	23.88	A	C
ATOM	5405	CG	LYS	696	74.230	62.883	59.891	1.00	27.19	A	C
ATOM	5406	CD	LYS	696	75.160	63.793	60.672	1.00	26.74	A	C
ATOM	5407	CE	LYS	696	76.354	64.211	59.816	1.00	26.44	A	C
ATOM	5408	NZ	LYS	696	77.248	65.163	60.534	1.00	28.88	A	N
ATOM	5409	C	LYS	696	71.256	60.670	60.962	1.00	24.58	A	C
ATOM	5410	O	LYS	696	71.673	59.790	61.710	1.00	24.47	A	O
ATOM	5411	N	GLN	697	69.986	61.060	60.949	1.00	24.66	A	N
ATOM	5412	CA	GLN	697	69.013	60.476	61.865	1.00	26.18	A	C
ATOM	5413	CB	GLN	697	68.072	61.571	62.385	1.00	28.53	A	C
ATOM	5414	CG	GLN	697	68.766	62.865	62.792	1.00	31.73	A	C
ATOM	5415	CD	GLN	697	67.790	63.938	63.262	1.00	34.90	A	C
ATOM	5416	OE1	GLN	697	68.086	65.133	63.195	1.00	37.16	A	O
ATOM	5417	NE2	GLN	697	66.627	63.516	63.753	1.00	36.42	A	N
ATOM	5418	C	GLN	697	68.176	59.346	61.259	1.00	24.79	A	C
ATOM	5419	O	GLN	697	67.294	58.808	61.923	1.00	27.00	A	O
ATOM	5420	N	VAL	698	68.439	58.979	60.011	1.00	21.46	A	N
ATOM	5421	CA	VAL	698	67.659	57.922	59.383	1.00	18.56	A	C
ATOM	5422	CB	VAL	698	66.510	58.517	58.524	1.00	19.77	A	C
ATOM	5423	CG1	VAL	698	65.674	59.467	59.355	1.00	19.11	A	C
ATOM	5424	CG2	VAL	698	67.077	59.233	57.296	1.00	15.74	A	C
ATOM	5425	C	VAL	698	68.469	56.987	58.484	1.00	18.57	A	C
ATOM	5426	O	VAL	698	69.614	57.265	58.135	1.00	17.50	A	O
ATOM	5427	N	GLU	699	67.850	55.868	58.121	1.00	18.32	A	N
ATOM	5428	CA	GLU	699	68.456	54.885	57.236	1.00	18.24	A	C
ATOM	5429	CB	GLU	699	68.007	53.488	57.636	1.00	19.38	A	C
ATOM	5430	CG	GLU	699	67.600	53.411	59.097	1.00	26.18	A	C
ATOM	5431	CD	GLU	699	68.384	52.377	59.891	1.00	29.91	A	C
ATOM	5432	OE1	GLU	699	69.620	52.305	59.712	1.00	31.51	A	O
ATOM	5433	OE2	GLU	699	67.765	51.651	60.703	1.00	30.28	A	O
ATOM	5434	C	GLU	699	67.857	55.286	55.891	1.00	17.20	A	C
ATOM	5435	O	GLU	699	66.638	55.397	55.765	1.00	16.35	A	O
ATOM	5436	N	TYR	700	68.714	55.516	54.899	1.00	15.53	A	N
ATOM	5437	CA	TYR	700	68.275	55.968	53.584	1.00	12.51	A	C
ATOM	5438	CB	TYR	700	68.810	57.383	53.365	1.00	12.28	A	C

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## FIG. 4 - 112

(Continued)

ATOM	5439	CG	TYR	700	68.374	58.105	52.114	1.00	13.03	A	C
ATOM	5440	CD1	TYR	700	67.027	58.171	51.746	1.00	12.78	A	C
ATOM	5441	CE1	TYR	700	66.611	58.961	50.666	1.00	7.94	A	C
ATOM	5442	CD2	TYR	700	69.301	58.840	51.359	1.00	12.91	A	C
ATOM	5443	CE2	TYR	700	68.895	59.629	50.282	1.00	10.45	A	C
ATOM	5444	CZ	TYR	700	67.550	59.688	49.948	1.00	10.05	A	C
ATOM	5445	OH	TYR	700	67.150	60.495	48.913	1.00	8.37	A	O
ATOM	5446	C	TYR	700	68.743	55.056	52.468	1.00	11.71	A	C
ATOM	5447	O	TYR	700	69.881	54.594	52.463	1.00	10.84	A	O
ATOM	5448	N	LEU	701	67.836	54.775	51.540	1.00	11.32	A	N
ATOM	5449	CA	LEU	701	68.142	53.950	50.383	1.00	11.03	A	C
ATOM	5450	CB	LEU	701	67.313	52.667	50.378	1.00	8.96	A	C
ATOM	5451	CG	LEU	701	67.439	51.794	49.123	1.00	10.04	A	C
ATOM	5452	CD1	LEU	701	68.841	51.873	48.511	1.00	7.25	A	C
ATOM	5453	CD2	LEU	701	67.089	50.376	49.490	1.00	5.44	A	C
ATOM	5454	C	LEU	701	67.811	54.799	49.170	1.00	13.03	A	C
ATOM	5455	O	LEU	701	66.660	55.219	48.986	1.00	13.35	A	O
ATOM	5456	N	LEU	702	68.840	55.068	48.367	1.00	12.91	A	N
ATOM	5457	CA	LEU	702	68.724	55.888	47.169	1.00	11.74	A	C
ATOM	5458	CB	LEU	702	69.806	56.968	47.196	1.00	11.17	A	C
ATOM	5459	CG	LEU	702	69.916	57.965	46.044	1.00	12.13	A	C
ATOM	5460	CD1	LEU	702	68.569	58.656	45.803	1.00	10.71	A	C
ATOM	5461	CD2	LEU	702	71.006	58.981	46.368	1.00	10.37	A	C
ATOM	5462	C	LEU	702	68.883	55.003	45.942	1.00	13.49	A	C
ATOM	5463	O	LEU	702	69.854	54.251	45.832	1.00	14.04	A	O
ATOM	5464	N	ILE	703	67.935	55.111	45.016	1.00	13.82	A	N
ATOM	5465	CA	ILE	703	67.934	54.297	43.806	1.00	12.92	A	C
ATOM	5466	CB	ILE	703	66.931	53.152	43.964	1.00	12.98	A	C
ATOM	5467	CG2	ILE	703	66.897	52.305	42.706	1.00	15.12	A	C
ATOM	5468	CG1	ILE	703	67.299	52.322	45.196	1.00	13.52	A	C
ATOM	5469	CD1	ILE	703	66.202	51.383	45.663	1.00	13.28	A	C
ATOM	5470	C	ILE	703	67.561	55.125	42.582	1.00	14.12	A	C
ATOM	5471	O	ILE	703	66.635	55.938	42.629	1.00	15.85	A	O
ATOM	5472	N	HIS	704	68.265	54.909	41.473	1.00	13.28	A	N
ATOM	5473	CA	HIS	704	67.987	55.678	40.265	1.00	11.81	A	C
ATOM	5474	CB	HIS	704	68.670	57.048	40.391	1.00	11.13	A	C
ATOM	5475	CG	HIS	704	67.968	58.156	39.667	1.00	11.66	A	C
ATOM	5476	CD2	HIS	704	67.446	58.221	38.418	1.00	10.83	A	C
ATOM	5477	ND1	HIS	704	67.736	59.387	40.244	1.00	10.07	A	N
ATOM	5478	CE1	HIS	704	67.098	60.162	39.385	1.00	9.04	A	C
ATOM	5479	NE2	HIS	704	66.910	59.479	38.270	1.00	11.23	A	N
ATOM	5480	C	HIS	704	68.464	54.965	38.992	1.00	11.87	A	C
ATOM	5481	O	HIS	704	69.503	54.306	38.980	1.00	11.87	A	O
ATOM	5482	N	GLY	705	67.684	55.082	37.926	1.00	11.49	A	N
ATOM	5483	CA	GLY	705	68.075	54.486	36.663	1.00	11.90	A	C
ATOM	5484	C	GLY	705	69.066	55.449	36.036	1.00	12.16	A	C
ATOM	5485	O	GLY	705	68.911	56.660	36.153	1.00	13.94	A	O
ATOM	5486	N	THR	706	70.086	54.928	35.372	1.00	13.29	A	N
ATOM	5487	CA	THR	706	71.101	55.782	34.770	1.00	12.51	A	C

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## FIG. 4 - 113

(Continued)

ATOM	5488	CB	THR	706	72.417	55.001	34.557	1.00	11.94	A	C
ATOM	5489	OG1	THR	706	72.230	53.983	33.565	1.00	12.79	A	O
ATOM	5490	CG2	THR	706	72.840	54.344	35.861	1.00	12.66	A	C
ATOM	5491	C	THR	706	70.678	56.409	33.455	1.00	13.02	A	C
ATOM	5492	O	THR	706	71.183	57.461	33.084	1.00	14.35	A	O
ATOM	5493	N	ALA	707	69.754	55.770	32.748	1.00	13.82	A	N
ATOM	5494	CA	ALA	707	69.289	56.302	31.469	1.00	15.26	A	C
ATOM	5495	CB	ALA	707	69.126	55.176	30.442	1.00	13.60	A	C
ATOM	5496	C	ALA	707	67.970	57.030	31.644	1.00	16.56	A	C
ATOM	5497	O	ALA	707	67.154	57.075	30.720	1.00	17.71	A	O
ATOM	5498	N	ASP	708	67.764	57.600	32.828	1.00	16.33	A	N
ATOM	5499	CA	ASP	708	66.534	58.314	33.113	1.00	16.71	A	C
ATOM	5500	CB	ASP	708	66.376	58.508	34.614	1.00	18.25	A	C
ATOM	5501	CG	ASP	708	64.957	58.834	35.000	1.00	19.59	A	C
ATOM	5502	OD1	ASP	708	64.304	59.612	34.266	1.00	18.82	A	O
ATOM	5503	OD2	ASP	708	64.498	58.317	36.038	1.00	19.68	A	O
ATOM	5504	C	ASP	708	66.490	59.673	32.408	1.00	17.30	A	C
ATOM	5505	O	ASP	708	67.131	60.647	32.843	1.00	18.75	A	O
ATOM	5506	N	ASP	709	65.715	59.722	31.327	1.00	13.98	A	N
ATOM	5507	CA	ASP	709	65.553	60.913	30.509	1.00	13.26	A	C
ATOM	5508	CB	ASP	709	65.028	60.503	29.137	1.00	11.83	A	C
ATOM	5509	CG	ASP	709	63.700	59.778	29.228	1.00	13.61	A	C
ATOM	5510	OD1	ASP	709	62.648	60.402	28.958	1.00	12.39	A	O
ATOM	5511	OD2	ASP	709	63.706	58.584	29.593	1.00	10.85	A	O
ATOM	5512	C	ASP	709	64.603	61.934	31.129	1.00	13.44	A	C
ATOM	5513	O	ASP	709	64.649	63.112	30.786	1.00	14.33	A	O
ATOM	5514	N	ASN	710	63.743	61.473	32.034	1.00	12.40	A	N
ATOM	5515	CA	ASN	710	62.761	62.331	32.702	1.00	11.63	A	C
ATOM	5516	CB	ASN	710	61.566	61.469	33.094	1.00	10.91	A	C
ATOM	5517	CG	ASN	710	60.388	62.276	33.572	1.00	12.77	A	C
ATOM	5518	OD1	ASN	710	59.271	61.760	33.651	1.00	14.18	A	O
ATOM	5519	ND2	ASN	710	60.621	63.539	33.903	1.00	12.05	A	N
ATOM	5520	C	ASN	710	63.395	63.010	33.938	1.00	13.10	A	C
ATOM	5521	O	ASN	710	63.691	64.211	33.912	1.00	12.53	A	O
ATOM	5522	N	VAL	711	63.570	62.246	35.017	1.00	11.10	A	N
ATOM	5523	CA	VAL	711	64.221	62.741	36.225	1.00	9.96	A	C
ATOM	5524	CB	VAL	711	63.620	62.128	37.512	1.00	9.85	A	C
ATOM	5525	CG1	VAL	711	64.415	62.570	38.719	1.00	7.61	A	C
ATOM	5526	CG2	VAL	711	62.176	62.567	37.675	1.00	11.26	A	C
ATOM	5527	C	VAL	711	65.645	62.237	36.038	1.00	10.48	A	C
ATOM	5528	O	VAL	711	65.949	61.068	36.280	1.00	10.00	A	O
ATOM	5529	N	HIS	712	66.518	63.126	35.591	1.00	10.94	A	N
ATOM	5530	CA	HIS	712	67.899	62.758	35.302	1.00	11.74	A	C
ATOM	5531	CB	HIS	712	68.577	63.961	34.646	1.00	10.79	A	C
ATOM	5532	CG	HIS	712	67.782	64.529	33.514	1.00	11.58	A	C
ATOM	5533	CD2	HIS	712	66.855	63.955	32.705	1.00	12.39	A	C
ATOM	5534	ND1	HIS	712	67.833	65.858	33.154	1.00	11.87	A	N
ATOM	5535	CE1	HIS	712	66.966	66.082	32.181	1.00	12.19	A	C
ATOM	5536	NE2	HIS	712	66.359	64.944	31.891	1.00	11.62	A	N

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## FIG. 4 - 114

(Continued)

ATOM	5537	C	HIS	712	68.698	62.222	36.491	1.00	10.63	A	C
ATOM	5538	O	HIS	712	68.461	62.598	37.633	1.00	11.98	A	O
ATOM	5539	N	PHE	713	69.631	61.319	36.210	1.00	10.82	A	N
ATOM	5540	CA	PHE	713	70.458	60.720	37.251	1.00	11.00	A	C
ATOM	5541	CB	PHE	713	71.533	59.823	36.634	1.00	11.14	A	C
ATOM	5542	CG	PHE	713	72.270	58.989	37.639	1.00	11.47	A	C
ATOM	5543	CD1	PHE	713	71.714	57.813	38.126	1.00	11.22	A	C
ATOM	5544	CD2	PHE	713	73.496	59.407	38.144	1.00	11.84	A	C
ATOM	5545	CE1	PHE	713	72.367	57.066	39.109	1.00	11.98	A	C
ATOM	5546	CE2	PHE	713	74.153	58.667	39.126	1.00	13.82	A	C
ATOM	5547	CZ	PHE	713	73.586	57.495	39.610	1.00	11.04	A	C
ATOM	5548	C	PHE	713	71.122	61.818	38.061	1.00	11.85	A	C
ATOM	5549	O	PHE	713	71.404	61.640	39.243	1.00	13.14	A	O
ATOM	5550	N	GLN	714	71.377	62.948	37.403	1.00	12.47	A	N
ATOM	5551	CA	GLN	714	72.001	64.113	38.022	1.00	10.55	A	C
ATOM	5552	CB	GLN	714	71.851	65.321	37.082	1.00	11.91	A	C
ATOM	5553	CG	GLN	714	72.055	66.695	37.740	1.00	10.69	A	C
ATOM	5554	CD	GLN	714	71.501	67.827	36.891	1.00	9.77	A	C
ATOM	5555	OE1	GLN	714	70.447	67.693	36.268	1.00	10.50	A	O
ATOM	5556	NE2	GLN	714	72.201	68.948	36.870	1.00	9.43	A	N
ATOM	5557	C	GLN	714	71.355	64.417	39.368	1.00	9.91	A	C
ATOM	5558	O	GLN	714	72.037	64.700	40.356	1.00	8.86	A	O
ATOM	5559	N	GLN	715	70.029	64.340	39.395	1.00	10.27	A	N
ATOM	5560	CA	GLN	715	69.255	64.616	40.599	1.00	10.62	A	C
ATOM	5561	CB	GLN	715	67.771	64.393	40.315	1.00	10.98	A	C
ATOM	5562	CG	GLN	715	67.267	65.219	39.144	1.00	11.10	A	C
ATOM	5563	CD	GLN	715	66.285	66.288	39.567	1.00	14.59	A	C
ATOM	5564	OE1	GLN	715	66.381	66.828	40.671	1.00	16.72	A	O
ATOM	5565	NE2	GLN	715	65.336	66.613	38.685	1.00	12.90	A	N
ATOM	5566	C	GLN	715	69.716	63.781	41.780	1.00	10.65	A	C
ATOM	5567	O	GLN	715	69.976	64.322	42.853	1.00	12.32	A	O
ATOM	5568	N	SER	716	69.828	62.472	41.600	1.00	9.91	A	N
ATOM	5569	CA	SER	716	70.299	61.630	42.700	1.00	12.35	A	C
ATOM	5570	CB	SER	716	69.937	60.163	42.461	1.00	10.77	A	C
ATOM	5571	OG	SER	716	68.541	59.994	42.492	1.00	14.60	A	O
ATOM	5572	C	SER	716	71.818	61.761	42.876	1.00	13.46	A	C
ATOM	5573	O	SER	716	72.341	61.556	43.976	1.00	14.90	A	O
ATOM	5574	N	ALA	717	72.522	62.094	41.797	1.00	12.22	A	N
ATOM	5575	CA	ALA	717	73.969	62.252	41.870	1.00	13.92	A	C
ATOM	5576	CB	ALA	717	74.555	62.487	40.479	1.00	12.46	A	C
ATOM	5577	C	ALA	717	74.299	63.423	42.790	1.00	13.73	A	C
ATOM	5578	O	ALA	717	75.257	63.375	43.560	1.00	15.24	A	O
ATOM	5579	N	GLN	718	73.504	64.482	42.710	1.00	13.27	A	N
ATOM	5580	CA	GLN	718	73.738	65.631	43.565	1.00	13.07	A	C
ATOM	5581	CB	GLN	718	72.976	66.841	43.035	1.00	13.93	A	C
ATOM	5582	CG	GLN	718	73.548	67.422	41.734	1.00	15.44	A	C
ATOM	5583	CD	GLN	718	74.996	67.865	41.867	1.00	13.84	A	C
ATOM	5584	OE1	GLN	718	75.467	68.172	42.950	1.00	16.85	A	O
ATOM	5585	NE2	GLN	718	75.699	67.915	40.755	1.00	17.86	A	N

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## FIG. 4 - 115

(Continued)

ATOM	5586	C	GLN	718	73.350	65.343	45.026	1.00	13.24	A	C
ATOM	5587	O	GLN	718	73.941	65.910	45.949	1.00	11.74	A	O
ATOM	5588	N	ILE	719	72.370	64.460	45.237	1.00	12.01	A	N
ATOM	5589	CA	ILE	719	71.956	64.110	46.594	1.00	11.94	A	C
ATOM	5590	CB	ILE	719	70.691	63.201	46.616	1.00	12.50	A	C
ATOM	5591	CG2	ILE	719	70.464	62.673	48.021	1.00	11.09	A	C
ATOM	5592	CG1	ILE	719	69.447	63.979	46.174	1.00	14.37	A	C
ATOM	5593	CD1	ILE	719	68.170	63.143	46.154	1.00	8.64	A	C
ATOM	5594	C	ILE	719	73.081	63.338	47.282	1.00	11.72	A	C
ATOM	5595	O	ILE	719	73.543	63.703	48.367	1.00	10.69	A	O
ATOM	5596	N	SER	720	73.508	62.262	46.632	1.00	11.35	A	N
ATOM	5597	CA	SER	720	74.557	61.405	47.155	1.00	11.02	A	C
ATOM	5598	CB	SER	720	74.901	60.325	46.135	1.00	10.89	A	C
ATOM	5599	OG	SER	720	75.471	60.894	44.970	1.00	13.75	A	O
ATOM	5600	C	SER	720	75.804	62.207	47.488	1.00	12.63	A	C
ATOM	5601	O	SER	720	76.429	61.995	48.537	1.00	11.68	A	O
ATOM	5602	N	LYS	721	76.159	63.129	46.594	1.00	12.18	A	N
ATOM	5603	CA	LYS	721	77.336	63.951	46.800	1.00	12.15	A	C
ATOM	5604	CB	LYS	721	77.613	64.823	45.571	1.00	11.24	A	C
ATOM	5605	CG	LYS	721	78.764	65.796	45.756	1.00	7.41	A	C
ATOM	5606	CD	LYS	721	79.517	66.064	44.451	1.00	9.30	A	C
ATOM	5607	CE	LYS	721	78.674	66.765	43.392	1.00	8.74	A	C
ATOM	5608	NZ	LYS	721	78.341	68.165	43.739	1.00	9.54	A	N
ATOM	5609	C	LYS	721	77.190	64.816	48.038	1.00	13.24	A	C
ATOM	5610	O	LYS	721	78.150	64.982	48.791	1.00	14.49	A	O
ATOM	5611	N	ALA	722	75.992	65.351	48.262	1.00	13.05	A	N
ATOM	5612	CA	ALA	722	75.760	66.198	49.432	1.00	13.21	A	C
ATOM	5613	CB	ALA	722	74.389	66.870	49.353	1.00	9.37	A	C
ATOM	5614	C	ALA	722	75.874	65.369	50.702	1.00	14.04	A	C
ATOM	5615	O	ALA	722	76.430	65.826	51.694	1.00	15.43	A	O
ATOM	5616	N	LEU	723	75.360	64.145	50.665	1.00	14.96	A	N
ATOM	5617	CA	LEU	723	75.429	63.266	51.826	1.00	17.23	A	C
ATOM	5618	CB	LEU	723	74.626	61.984	51.570	1.00	16.86	A	C
ATOM	5619	CG	LEU	723	73.116	62.205	51.463	1.00	18.78	A	C
ATOM	5620	CD1	LEU	723	72.428	60.932	50.991	1.00	18.74	A	C
ATOM	5621	CD2	LEU	723	72.576	62.663	52.817	1.00	16.86	A	C
ATOM	5622	C	LEU	723	76.889	62.926	52.134	1.00	17.26	A	C
ATOM	5623	O	LEU	723	77.320	62.990	53.280	1.00	18.48	A	O
ATOM	5624	N	VAL	724	77.641	62.559	51.103	1.00	17.41	A	N
ATOM	5625	CA	VAL	724	79.050	62.234	51.257	1.00	16.64	A	C
ATOM	5626	CB	VAL	724	79.671	61.824	49.902	1.00	14.31	A	C
ATOM	5627	CG1	VAL	724	81.187	61.819	49.987	1.00	13.56	A	C
ATOM	5628	CG2	VAL	724	79.178	60.449	49.519	1.00	14.78	A	C
ATOM	5629	C	VAL	724	79.785	63.455	51.803	1.00	18.83	A	C
ATOM	5630	O	VAL	724	80.665	63.337	52.662	1.00	19.09	A	O
ATOM	5631	N	ASP	725	79.411	64.632	51.318	1.00	19.19	A	N
ATOM	5632	CA	ASP	725	80.051	65.848	51.776	1.00	20.26	A	C
ATOM	5633	CB	ASP	725	79.627	67.032	50.919	1.00	22.40	A	C
ATOM	5634	CG	ASP	725	80.259	67.004	49.549	1.00	26.44	A	C

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(Continued)

## FIG. 4 - 116

ATOM	5635	OD1	ASP	725	81.149	66.151	49.319	1.00	26.28	A	O
ATOM	5636	OD2	ASP	725	79.867	67.839	48.704	1.00	30.70	A	O
ATOM	5637	C	ASP	725	79.805	66.171	53.238	1.00	19.86	A	C
ATOM	5638	O	ASP	725	80.486	67.024	53.792	1.00	23.33	A	O
ATOM	5639	N	VAL	726	78.841	65.516	53.873	1.00	17.95	A	N
ATOM	5640	CA	VAL	726	78.603	65.790	55.285	1.00	17.97	A	C
ATOM	5641	CB	VAL	726	77.178	66.341	55.567	1.00	18.54	A	C
ATOM	5642	CG1	VAL	726	76.992	67.680	54.875	1.00	16.64	A	C
ATOM	5643	CG2	VAL	726	76.121	65.339	55.120	1.00	18.24	A	C
ATOM	5644	C	VAL	726	78.812	64.549	56.124	1.00	17.82	A	C
ATOM	5645	O	VAL	726	78.412	64.504	57.283	1.00	19.86	A	O
ATOM	5646	N	GLY	727	79.439	63.541	55.535	1.00	17.13	A	N
ATOM	5647	CA	GLY	727	79.711	62.317	56.263	1.00	16.84	A	C
ATOM	5648	C	GLY	727	78.509	61.489	56.681	1.00	17.94	A	C
ATOM	5649	O	GLY	727	78.483	60.961	57.794	1.00	19.74	A	O
ATOM	5650	N	VAL	728	77.517	61.371	55.802	1.00	16.62	A	N
ATOM	5651	CA	VAL	728	76.331	60.571	56.085	1.00	17.26	A	C
ATOM	5652	CB	VAL	728	75.030	61.302	55.643	1.00	18.46	A	C
ATOM	5653	CG1	VAL	728	73.838	60.338	55.668	1.00	16.22	A	C
ATOM	5654	CG2	VAL	728	74.753	62.476	56.579	1.00	18.70	A	C
ATOM	5655	C	VAL	728	76.411	59.230	55.347	1.00	18.03	A	C
ATOM	5656	O	VAL	728	76.667	59.186	54.143	1.00	18.40	A	O
ATOM	5657	N	ASP	729	76.211	58.135	56.069	1.00	18.22	A	N
ATOM	5658	CA	ASP	729	76.246	56.822	55.441	1.00	19.90	A	C
ATOM	5659	CB	ASP	729	76.734	55.752	56.420	1.00	22.57	A	C
ATOM	5660	CG	ASP	729	76.819	54.376	55.778	1.00	25.97	A	C
ATOM	5661	OD1	ASP	729	77.340	54.278	54.649	1.00	27.13	A	O
ATOM	5662	OD2	ASP	729	76.372	53.388	56.398	1.00	30.03	A	O
ATOM	5663	C	ASP	729	74.839	56.504	54.984	1.00	19.16	A	C
ATOM	5664	O	ASP	729	73.868	56.863	55.649	1.00	21.91	A	O
ATOM	5665	N	PHE	730	74.723	55.838	53.846	1.00	18.27	A	N
ATOM	5666	CA	PHE	730	73.416	55.499	53.299	1.00	16.06	A	C
ATOM	5667	CB	PHE	730	72.796	56.734	52.639	1.00	14.49	A	C
ATOM	5668	CG	PHE	730	73.590	57.265	51.480	1.00	12.02	A	C
ATOM	5669	CD1	PHE	730	73.262	56.913	50.177	1.00	10.26	A	C
ATOM	5670	CD2	PHE	730	74.691	58.082	51.694	1.00	11.55	A	C
ATOM	5671	CE1	PHE	730	74.020	57.364	49.098	1.00	10.41	A	C
ATOM	5672	CE2	PHE	730	75.459	58.537	50.621	1.00	13.40	A	C
ATOM	5673	CZ	PHE	730	75.120	58.175	49.317	1.00	9.85	A	C
ATOM	5674	C	PHE	730	73.565	54.388	52.281	1.00	16.20	A	C
ATOM	5675	O	PHE	730	74.675	53.990	51.945	1.00	18.49	A	O
ATOM	5676	N	GLN	731	72.447	53.883	51.791	1.00	17.40	A	N
ATOM	5677	CA	GLN	731	72.484	52.813	50.813	1.00	17.82	A	C
ATOM	5678	CB	GLN	731	71.514	51.708	51.208	1.00	20.04	A	C
ATOM	5679	CG	GLN	731	71.641	51.257	52.644	1.00	25.37	A	C
ATOM	5680	CD	GLN	731	73.019	50.737	52.968	1.00	28.25	A	C
ATOM	5681	OE1	GLN	731	73.554	49.883	52.256	1.00	32.85	A	O
ATOM	5682	NE2	GLN	731	73.603	51.238	54.055	1.00	30.12	A	N
ATOM	5683	C	GLN	731	72.091	53.382	49.458	1.00	17.65	A	C

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## FIG. 4 - 117

(Continued)

ATOM	5684	O	GLN	731	71.160	54.191	49.355	1.00	17.02	A	O
ATOM	5685	N	ALA	732	72.802	52.962	48.421	1.00	14.78	A	N
ATOM	5686	CA	ALA	732	72.510	53.444	47.088	1.00	15.21	A	C
ATOM	5687	CB	ALA	732	73.588	54.409	46.626	1.00	15.17	A	C
ATOM	5688	C	ALA	732	72.419	52.282	46.131	1.00	15.21	A	C
ATOM	5689	O	ALA	732	72.940	51.207	46.396	1.00	16.17	A	O
ATOM	5690	N	MET	733	71.737	52.504	45.019	1.00	14.57	A	N
ATOM	5691	CA	MET	733	71.599	51.483	44.008	1.00	14.86	A	C
ATOM	5692	CB	MET	733	70.490	50.499	44.383	1.00	15.14	A	C
ATOM	5693	CG	MET	733	70.288	49.386	43.353	1.00	18.04	A	C
ATOM	5694	SD	MET	733	71.814	48.476	42.961	1.00	22.04	A	S
ATOM	5695	CE	MET	733	71.892	47.307	44.310	1.00	17.75	A	C
ATOM	5696	C	MET	733	71.283	52.153	42.683	1.00	14.93	A	C
ATOM	5697	O	MET	733	70.317	52.915	42.574	1.00	13.98	A	O
ATOM	5698	N	TRP	734	72.113	51.884	41.680	1.00	13.82	A	N
ATOM	5699	CA	TRP	734	71.890	52.447	40.356	1.00	13.13	A	C
ATOM	5700	CB	TRP	734	73.173	53.117	39.827	1.00	10.39	A	C
ATOM	5701	CG	TRP	734	74.187	52.159	39.267	1.00	8.77	A	C
ATOM	5702	CD2	TRP	734	75.398	51.726	39.894	1.00	7.74	A	C
ATOM	5703	CE2	TRP	734	75.984	50.757	39.053	1.00	9.97	A	C
ATOM	5704	CE3	TRP	734	76.045	52.062	41.087	1.00	8.70	A	C
ATOM	5705	CD1	TRP	734	74.095	51.463	38.095	1.00	10.56	A	C
ATOM	5706	NE1	TRP	734	75.170	50.613	37.961	1.00	12.87	A	N
ATOM	5707	CZ2	TRP	734	77.183	50.119	39.369	1.00	9.94	A	C
ATOM	5708	CZ3	TRP	734	77.238	51.428	41.400	1.00	9.32	A	C
ATOM	5709	CH2	TRP	734	77.793	50.468	40.545	1.00	9.49	A	C
ATOM	5710	C	TRP	734	71.480	51.291	39.445	1.00	14.06	A	C
ATOM	5711	O	TRP	734	71.903	50.155	39.653	1.00	13.91	A	O
ATOM	5712	N	TYR	735	70.635	51.570	38.461	1.00	15.15	A	N
ATOM	5713	CA	TYR	735	70.223	50.544	37.504	1.00	15.51	A	C
ATOM	5714	CB	TYR	735	68.705	50.326	37.556	1.00	14.10	A	C
ATOM	5715	CG	TYR	735	68.300	49.439	38.709	1.00	14.76	A	C
ATOM	5716	CD1	TYR	735	68.619	48.081	38.708	1.00	14.45	A	C
ATOM	5717	CE1	TYR	735	68.360	47.278	39.816	1.00	14.33	A	C
ATOM	5718	CD2	TYR	735	67.696	49.971	39.848	1.00	15.84	A	C
ATOM	5719	CE2	TYR	735	67.432	49.180	40.960	1.00	14.52	A	C
ATOM	5720	CZ	TYR	735	67.772	47.835	40.938	1.00	16.33	A	C
ATOM	5721	OH	TYR	735	67.547	47.056	42.048	1.00	17.53	A	O
ATOM	5722	C	TYR	735	70.685	50.966	36.104	1.00	16.31	A	C
ATOM	5723	O	TYR	735	70.103	51.858	35.466	1.00	15.82	A	O
ATOM	5724	N	THR	736	71.763	50.330	35.654	1.00	15.44	A	N
ATOM	5725	CA	THR	736	72.361	50.608	34.353	1.00	15.13	A	C
ATOM	5726	CB	THR	736	73.491	49.602	34.030	1.00	14.68	A	C
ATOM	5727	OG1	THR	736	74.470	49.614	35.076	1.00	15.48	A	O
ATOM	5728	CG2	THR	736	74.156	49.961	32.713	1.00	14.72	A	C
ATOM	5729	C	THR	736	71.365	50.549	33.206	1.00	15.41	A	C
ATOM	5730	O	THR	736	70.650	49.560	33.044	1.00	16.44	A	O
ATOM	5731	N	ASP	737	71.335	51.614	32.414	1.00	15.92	A	N
ATOM	5732	CA	ASP	737	70.475	51.719	31.238	1.00	16.48	A	C

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## FIG. 4 - 118

(Continued)

ATOM	5733	CB	ASP	737	70.884	50.677	30.200	1.00	15.90	A	C
ATOM	5734	CG	ASP	737	72.232	50.972	29.574	1.00	20.37	A	C
ATOM	5735	OD1	ASP	737	72.679	50.147	28.747	1.00	24.29	A	O
ATOM	5736	OD2	ASP	737	72.847	52.020	29.895	1.00	18.74	A	O
ATOM	5737	C	ASP	737	68.974	51.632	31.467	1.00	17.71	A	C
ATOM	5738	O	ASP	737	68.205	51.507	30.515	1.00	18.86	A	O
ATOM	5739	N	GLU	738	68.553	51.692	32.722	1.00	18.39	A	N
ATOM	5740	CA	GLU	738	67.135	51.644	33.033	1.00	19.00	A	C
ATOM	5741	CB	GLU	738	66.909	50.999	34.407	1.00	20.24	A	C
ATOM	5742	CG	GLU	738	66.904	49.485	34.380	1.00	20.93	A	C
ATOM	5743	CD	GLU	738	65.741	48.937	33.565	1.00	24.58	A	C
ATOM	5744	OE1	GLU	738	64.588	49.289	33.878	1.00	27.21	A	O
ATOM	5745	OE2	GLU	738	65.970	48.163	32.611	1.00	26.16	A	O
ATOM	5746	C	GLU	738	66.624	53.076	33.025	1.00	19.38	A	C
ATOM	5747	O	GLU	738	67.327	53.991	33.461	1.00	20.83	A	O
ATOM	5748	N	ASP	739	65.414	53.288	32.525	1.00	18.55	A	N
ATOM	5749	CA	ASP	739	64.892	54.642	32.493	1.00	17.49	A	C
ATOM	5750	CB	ASP	739	64.074	54.863	31.222	1.00	18.32	A	C
ATOM	5751	CG	ASP	739	62.689	54.271	31.293	1.00	21.44	A	C
ATOM	5752	OD1	ASP	739	61.995	54.340	30.257	1.00	24.73	A	O
ATOM	5753	OD2	ASP	739	62.285	53.752	32.358	1.00	21.35	A	O
ATOM	5754	C	ASP	739	64.088	54.976	33.750	1.00	17.35	A	C
ATOM	5755	O	ASP	739	64.191	54.282	34.762	1.00	15.74	A	O
ATOM	5756	N	HIS	740	63.291	56.034	33.687	1.00	16.96	A	N
ATOM	5757	CA	HIS	740	62.521	56.469	34.842	1.00	18.24	A	C
ATOM	5758	CB	HIS	740	61.746	57.736	34.511	1.00	16.88	A	C
ATOM	5759	CG	HIS	740	61.145	58.392	35.710	1.00	17.57	A	C
ATOM	5760	CD2	HIS	740	59.883	58.812	35.961	1.00	16.26	A	C
ATOM	5761	ND1	HIS	740	61.881	58.687	36.837	1.00	17.31	A	N
ATOM	5762	CE1	HIS	740	61.097	59.262	37.732	1.00	18.51	A	C
ATOM	5763	NE2	HIS	740	59.880	59.349	37.224	1.00	17.94	A	N
ATOM	5764	C	HIS	740	61.557	55.449	35.426	1.00	19.90	A	C
ATOM	5765	O	HIS	740	61.191	55.539	36.599	1.00	20.00	A	O
ATOM	5766	N	GLY	741	61.151	54.481	34.614	1.00	19.40	A	N
ATOM	5767	CA	GLY	741	60.216	53.484	35.084	1.00	18.82	A	C
ATOM	5768	C	GLY	741	60.849	52.218	35.609	1.00	20.36	A	C
ATOM	5769	O	GLY	741	60.165	51.404	36.237	1.00	22.79	A	O
ATOM	5770	N	ILE	742	62.145	52.045	35.368	1.00	19.61	A	N
ATOM	5771	CA	ILE	742	62.854	50.849	35.821	1.00	17.74	A	C
ATOM	5772	CB	ILE	742	63.273	50.981	37.294	1.00	14.46	A	C
ATOM	5773	CG2	ILE	742	64.279	49.917	37.638	1.00	14.37	A	C
ATOM	5774	CG1	ILE	742	63.865	52.370	37.540	1.00	13.43	A	C
ATOM	5775	CD1	ILE	742	64.540	52.552	38.887	1.00	9.55	A	C
ATOM	5776	C	ILE	742	61.907	49.658	35.676	1.00	19.11	A	C
ATOM	5777	O	ILE	742	61.805	48.825	36.571	1.00	18.97	A	O
ATOM	5778	N	ALA	743	61.217	49.594	34.534	1.00	20.16	A	N
ATOM	5779	CA	ALA	743	60.246	48.538	34.268	1.00	19.71	A	C
ATOM	5780	CB	ALA	743	59.004	49.141	33.630	1.00	19.65	A	C
ATOM	5781	C	ALA	743	60.717	47.350	33.430	1.00	20.08	A	C

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## FIG. 4 - 119

(Continued)

ATOM	5782	O	ALA	743	59.898	46.536	33.006	1.00	20.99	A	O
ATOM	5783	N	SER	744	62.009	47.230	33.163	1.00	19.12	A	N
ATOM	5784	CA	SER	744	62.438	46.074	32.389	1.00	17.34	A	C
ATOM	5785	CB	SER	744	63.931	46.132	32.068	1.00	14.62	A	C
ATOM	5786	OG	SER	744	64.699	45.597	33.125	1.00	18.04	A	O
ATOM	5787	C	SER	744	62.132	44.896	33.300	1.00	16.58	A	C
ATOM	5788	O	SER	744	62.137	45.032	34.519	1.00	15.47	A	O
ATOM	5789	N	SER	745	61.853	43.742	32.715	1.00	19.10	A	N
ATOM	5790	CA	SER	745	61.524	42.558	33.503	1.00	20.03	A	C
ATOM	5791	CB	SER	745	61.417	41.343	32.598	1.00	20.12	A	C
ATOM	5792	OG	SER	745	61.110	40.209	33.377	1.00	27.90	A	O
ATOM	5793	C	SER	745	62.510	42.245	34.624	1.00	19.80	A	C
ATOM	5794	O	SER	745	62.130	42.078	35.781	1.00	19.78	A	O
ATOM	5795	N	THR	746	63.783	42.158	34.277	1.00	19.56	A	N
ATOM	5796	CA	THR	746	64.796	41.849	35.265	1.00	19.48	A	C
ATOM	5797	CB	THR	746	66.125	41.538	34.575	1.00	20.06	A	C
ATOM	5798	OG1	THR	746	66.463	42.615	33.691	1.00	23.41	A	O
ATOM	5799	CG2	THR	746	66.009	40.259	33.772	1.00	16.20	A	C
ATOM	5800	C	THR	746	64.996	42.966	36.288	1.00	19.59	A	C
ATOM	5801	O	THR	746	65.066	42.706	37.488	1.00	20.63	A	O
ATOM	5802	N	ALA	747	65.070	44.208	35.821	1.00	18.73	A	N
ATOM	5803	CA	ALA	747	65.286	45.334	36.723	1.00	18.03	A	C
ATOM	5804	CB	ALA	747	65.554	46.609	35.919	1.00	15.38	A	C
ATOM	5805	C	ALA	747	64.113	45.540	37.681	1.00	17.35	A	C
ATOM	5806	O	ALA	747	64.291	45.989	38.814	1.00	18.52	A	O
ATOM	5807	N	HIS	748	62.915	45.206	37.224	1.00	16.75	A	N
ATOM	5808	CA	HIS	748	61.718	45.342	38.046	1.00	16.92	A	C
ATOM	5809	CB	HIS	748	60.477	45.005	37.220	1.00	13.48	A	C
ATOM	5810	CG	HIS	748	59.214	44.968	38.020	1.00	14.10	A	C
ATOM	5811	CD2	HIS	748	58.397	43.941	38.348	1.00	12.63	A	C
ATOM	5812	ND1	HIS	748	58.663	46.094	38.595	1.00	14.71	A	N
ATOM	5813	CE1	HIS	748	57.561	45.762	39.241	1.00	13.05	A	C
ATOM	5814	NE2	HIS	748	57.377	44.461	39.107	1.00	14.46	A	N
ATOM	5815	C	HIS	748	61.790	44.415	39.263	1.00	18.16	A	C
ATOM	5816	O	HIS	748	61.525	44.816	40.394	1.00	20.72	A	O
ATOM	5817	N	GLN	749	62.148	43.165	39.025	1.00	18.81	A	N
ATOM	5818	CA	GLN	749	62.241	42.201	40.105	1.00	19.53	A	C
ATOM	5819	CB	GLN	749	62.408	40.801	39.519	1.00	20.05	A	C
ATOM	5820	CG	GLN	749	61.291	40.428	38.550	1.00	21.82	A	C
ATOM	5821	CD	GLN	749	61.618	39.190	37.757	1.00	20.87	A	C
ATOM	5822	OE1	GLN	749	62.047	38.187	38.316	1.00	22.37	A	O
ATOM	5823	NE2	GLN	749	61.415	39.249	36.447	1.00	20.00	A	N
ATOM	5824	C	GLN	749	63.416	42.524	41.008	1.00	19.07	A	C
ATOM	5825	O	GLN	749	63.335	42.388	42.231	1.00	17.88	A	O
ATOM	5826	N	HIS	750	64.508	42.972	40.399	1.00	18.97	A	N
ATOM	5827	CA	HIS	750	65.707	43.275	41.160	1.00	16.68	A	C
ATOM	5828	CB	HIS	750	66.871	43.597	40.226	1.00	14.65	A	C
ATOM	5829	CG	HIS	750	68.208	43.496	40.889	1.00	13.97	A	C
ATOM	5830	CD2	HIS	750	69.207	42.593	40.749	1.00	12.94	A	C

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## FIG. 4 - 120

(Continued)

ATOM	5831	ND1	HIS	750	68.615	44.365	41.877	1.00	13.54	A	N
ATOM	5832	CE1	HIS	750	69.804	44.000	42.320	1.00	12.57	A	C
ATOM	5833	NE2	HIS	750	70.185	42.927	41.653	1.00	12.04	A	N
ATOM	5834	C	HIS	750	65.529	44.400	42.157	1.00	17.33	A	C
ATOM	5835	O	HIS	750	65.945	44.277	43.309	1.00	18.09	A	O
ATOM	5836	N	ILE	751	64.899	45.490	41.726	1.00	17.03	A	N
ATOM	5837	CA	ILE	751	64.704	46.632	42.604	1.00	15.90	A	C
ATOM	5838	CB	ILE	751	64.206	47.849	41.805	1.00	17.60	A	C
ATOM	5839	CG2	ILE	751	62.893	47.504	41.088	1.00	16.17	A	C
ATOM	5840	CG1	ILE	751	64.065	49.058	42.736	1.00	15.94	A	C
ATOM	5841	CD1	ILE	751	63.684	50.332	42.017	1.00	12.51	A	C
ATOM	5842	C	ILE	751	63.751	46.341	43.767	1.00	16.09	A	C
ATOM	5843	O	ILE	751	64.062	46.632	44.919	1.00	16.37	A	O
ATOM	5844	N	TYR	752	62.596	45.759	43.480	1.00	16.32	A	N
ATOM	5845	CA	TYR	752	61.651	45.449	44.551	1.00	16.16	A	C
ATOM	5846	CB	TYR	752	60.323	44.967	43.968	1.00	13.79	A	C
ATOM	5847	CG	TYR	752	59.443	46.126	43.593	1.00	12.59	A	C
ATOM	5848	CD1	TYR	752	58.840	46.899	44.580	1.00	11.61	A	C
ATOM	5849	CE1	TYR	752	58.102	48.026	44.258	1.00	9.67	A	C
ATOM	5850	CD2	TYR	752	59.279	46.510	42.260	1.00	12.75	A	C
ATOM	5851	CE2	TYR	752	58.543	47.644	41.930	1.00	10.28	A	C
ATOM	5852	CZ	TYR	752	57.964	48.395	42.940	1.00	9.02	A	C
ATOM	5853	OH	TYR	752	57.278	49.542	42.642	1.00	12.10	A	O
ATOM	5854	C	TYR	752	62.226	44.429	45.522	1.00	16.42	A	C
ATOM	5855	O	TYR	752	61.927	44.467	46.719	1.00	16.42	A	O
ATOM	5856	N	THR	753	63.056	43.526	45.004	1.00	15.74	A	N
ATOM	5857	CA	THR	753	63.700	42.521	45.835	1.00	16.30	A	C
ATOM	5858	CB	THR	753	64.502	41.510	44.985	1.00	15.57	A	C
ATOM	5859	OG1	THR	753	63.601	40.677	44.253	1.00	15.74	A	O
ATOM	5860	CG2	THR	753	65.385	40.641	45.870	1.00	10.01	A	C
ATOM	5861	C	THR	753	64.678	43.240	46.758	1.00	18.17	A	C
ATOM	5862	O	THR	753	64.788	42.923	47.941	1.00	19.02	A	O
ATOM	5863	N	HIS	754	65.388	44.215	46.199	1.00	18.78	A	N
ATOM	5864	CA	HIS	754	66.363	44.972	46.959	1.00	18.90	A	C
ATOM	5865	CB	HIS	754	67.189	45.857	46.023	1.00	19.13	A	C
ATOM	5866	CG	HIS	754	68.449	46.379	46.644	1.00	19.62	A	C
ATOM	5867	CD2	HIS	754	68.786	47.619	47.070	1.00	18.70	A	C
ATOM	5868	ND1	HIS	754	69.539	45.576	46.904	1.00	18.44	A	N
ATOM	5869	CE1	HIS	754	70.493	46.298	47.462	1.00	17.52	A	C
ATOM	5870	NE2	HIS	754	70.062	47.541	47.574	1.00	19.51	A	N
ATOM	5871	C	HIS	754	65.663	45.828	48.007	1.00	19.38	A	C
ATOM	5872	O	HIS	754	66.088	45.876	49.158	1.00	19.63	A	O
ATOM	5873	N	MET	755	64.589	46.502	47.615	1.00	18.83	A	N
ATOM	5874	CA	MET	755	63.854	47.342	48.558	1.00	19.68	A	C
ATOM	5875	CB	MET	755	62.758	48.136	47.839	1.00	16.86	A	C
ATOM	5876	CG	MET	755	63.283	49.173	46.876	1.00	16.00	A	C
ATOM	5877	SD	MET	755	62.016	50.314	46.309	1.00	20.78	A	S
ATOM	5878	CE	MET	755	61.100	49.270	45.200	1.00	15.61	A	C
ATOM	5879	C	MET	755	63.232	46.506	49.676	1.00	20.27	A	C

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## FIG. 4 - 1 2 1

(Continued)

ATOM	5880	O	MET	755	63.112	46.969	50.811	1.00	20.56	A	O
ATOM	5881	N	SER	756	62.842	45.276	49.352	1.00	20.59	A	N
ATOM	5882	CA	SER	756	62.240	44.380	50.332	1.00	21.43	A	C
ATOM	5883	CB	SER	756	61.740	43.106	49.646	1.00	21.74	A	C
ATOM	5884	OG	SER	756	60.598	43.373	48.850	1.00	21.68	A	O
ATOM	5885	C	SER	756	63.224	44.023	51.444	1.00	22.50	A	C
ATOM	5886	O	SER	756	62.858	44.022	52.623	1.00	22.47	A	O
ATOM	5887	N	HIS	757	64.466	43.716	51.073	1.00	22.47	A	N
ATOM	5888	CA	HIS	757	65.483	43.384	52.065	1.00	23.01	A	C
ATOM	5889	CB	HIS	757	66.828	43.032	51.407	1.00	21.90	A	C
ATOM	5890	CG	HIS	757	66.837	41.721	50.682	1.00	24.99	A	C
ATOM	5891	CD2	HIS	757	67.344	41.375	49.473	1.00	26.07	A	C
ATOM	5892	ND1	HIS	757	66.314	40.563	51.220	1.00	26.51	A	N
ATOM	5893	CE1	HIS	757	66.497	39.564	50.375	1.00	25.15	A	C
ATOM	5894	NE2	HIS	757	67.120	40.029	49.307	1.00	25.93	A	N
ATOM	5895	C	HIS	757	65.689	44.596	52.966	1.00	23.03	A	C
ATOM	5896	O	HIS	757	65.823	44.474	54.186	1.00	24.03	A	O
ATOM	5897	N	PHE	758	65.704	45.771	52.356	1.00	22.28	A	N
ATOM	5898	CA	PHE	758	65.920	46.995	53.106	1.00	24.10	A	C
ATOM	5899	CB	PHE	758	66.005	48.190	52.161	1.00	20.12	A	C
ATOM	5900	CG	PHE	758	66.455	49.448	52.828	1.00	17.08	A	C
ATOM	5901	CD1	PHE	758	67.803	49.657	53.106	1.00	15.49	A	C
ATOM	5902	CD2	PHE	758	65.537	50.429	53.176	1.00	15.44	A	C
ATOM	5903	CE1	PHE	758	68.233	50.825	53.717	1.00	14.07	A	C
ATOM	5904	CE2	PHE	758	65.955	51.607	53.789	1.00	17.18	A	C
ATOM	5905	CZ	PHE	758	67.308	51.806	54.060	1.00	15.05	A	C
ATOM	5906	C	PHE	758	64.832	47.254	54.135	1.00	26.28	A	C
ATOM	5907	O	PHE	758	65.120	47.546	55.295	1.00	28.09	A	O
ATOM	5908	N	ILE	759	63.580	47.162	53.706	1.00	27.69	A	N
ATOM	5909	CA	ILE	759	62.461	47.394	54.605	1.00	29.02	A	C
ATOM	5910	CB	ILE	759	61.129	47.271	53.853	1.00	28.24	A	C
ATOM	5911	CG2	ILE	759	59.967	47.207	54.836	1.00	29.09	A	C
ATOM	5912	CG1	ILE	759	60.990	48.446	52.884	1.00	28.85	A	C
ATOM	5913	CD1	ILE	759	61.173	49.809	53.535	1.00	27.28	A	C
ATOM	5914	C	ILE	759	62.467	46.420	55.774	1.00	31.10	A	C
ATOM	5915	O	ILE	759	62.292	46.822	56.925	1.00	30.20	A	O
ATOM	5916	N	LYS	760	62.669	45.140	55.464	1.00	32.71	A	N
ATOM	5917	CA	LYS	760	62.697	44.079	56.465	1.00	33.04	A	C
ATOM	5918	CB	LYS	760	62.732	42.715	55.780	1.00	34.00	A	C
ATOM	5919	CG	LYS	760	61.405	42.300	55.164	1.00	37.68	A	C
ATOM	5920	CD	LYS	760	61.620	41.455	53.916	1.00	40.82	A	C
ATOM	5921	CE	LYS	760	62.473	40.229	54.199	1.00	42.70	A	C
ATOM	5922	NZ	LYS	760	62.952	39.600	52.933	1.00	44.73	A	N
ATOM	5923	C	LYS	760	63.885	44.205	57.396	1.00	33.20	A	C
ATOM	5924	O	LYS	760	63.874	43.676	58.504	1.00	34.38	A	O
ATOM	5925	N	GLN	761	64.914	44.902	56.939	1.00	33.26	A	N
ATOM	5926	CA	GLN	761	66.106	45.100	57.744	1.00	33.22	A	C
ATOM	5927	CB	GLN	761	67.295	45.422	56.830	1.00	35.03	A	C
ATOM	5928	CG	GLN	761	68.638	45.584	57.525	1.00	38.28	A	C

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## FIG. 4 - 122

(Continued)

ATOM	5929	CD	GLN	761	68.759	46.893	58.283	1.00	42.12	A	C
ATOM	5930	OE1	GLN	761	68.487	47.969	57.739	1.00	43.62	A	O
ATOM	5931	NE2	GLN	761	69.177	46.811	59.544	1.00	44.19	A	N
ATOM	5932	C	GLN	761	65.819	46.251	58.701	1.00	32.55	A	C
ATOM	5933	O	GLN	761	66.064	46.149	59.898	1.00	32.49	A	O
ATOM	5934	N	CYS	762	65.276	47.337	58.161	1.00	32.03	A	N
ATOM	5935	CA	CYS	762	64.945	48.513	58.953	1.00	33.26	A	C
ATOM	5936	C	CYS	762	63.888	48.216	60.023	1.00	32.69	A	C
ATOM	5937	O	CYS	762	63.892	48.830	61.087	1.00	32.22	A	O
ATOM	5938	CB	CYS	762	64.470	49.643	58.025	1.00	33.90	A	C
ATOM	5939	SG	CYS	762	63.606	51.029	58.843	1.00	40.21	A	S
ATOM	5940	N	PHE	763	62.993	47.271	59.742	1.00	32.59	A	N
ATOM	5941	CA	PHE	763	61.948	46.907	60.694	1.00	34.25	A	C
ATOM	5942	CB	PHE	763	60.618	46.647	59.981	1.00	31.61	A	C
ATOM	5943	CG	PHE	763	59.919	47.892	59.525	1.00	30.04	A	C
ATOM	5944	CD1	PHE	763	60.371	49.148	59.923	1.00	29.45	A	C
ATOM	5945	CD2	PHE	763	58.800	47.808	58.703	1.00	28.65	A	C
ATOM	5946	CE1	PHE	763	59.718	50.300	59.510	1.00	29.27	A	C
ATOM	5947	CE2	PHE	763	58.139	48.951	58.284	1.00	28.76	A	C
ATOM	5948	CZ	PHE	763	58.598	50.202	58.688	1.00	30.54	A	C
ATOM	5949	C	PHE	763	62.293	45.688	61.535	1.00	36.77	A	C
ATOM	5950	O	PHE	763	61.499	45.276	62.381	1.00	36.29	A	O
ATOM	5951	N	SER	764	63.463	45.102	61.290	1.00	39.62	A	N
ATOM	5952	CA	SER	764	63.907	43.941	62.052	1.00	43.05	A	C
ATOM	5953	CB	SER	764	65.356	43.598	61.701	1.00	44.44	A	C
ATOM	5954	OG	SER	764	66.215	44.709	61.913	1.00	48.06	A	O
ATOM	5955	C	SER	764	63.799	44.314	63.522	1.00	45.02	A	C
ATOM	5956	O	SER	764	64.195	45.412	63.916	1.00	44.75	A	O
ATOM	5957	N	LEU	765	63.264	43.412	64.335	1.00	48.04	A	N
ATOM	5958	CA	LEU	765	63.092	43.716	65.747	1.00	51.59	A	C
ATOM	5959	CB	LEU	765	61.624	44.067	66.017	1.00	50.97	A	C
ATOM	5960	CG	LEU	765	61.332	44.846	67.299	1.00	50.79	A	C
ATOM	5961	CD1	LEU	765	61.996	46.215	67.221	1.00	50.85	A	C
ATOM	5962	CD2	LEU	765	59.834	44.996	67.481	1.00	50.72	A	C
ATOM	5963	C	LEU	765	63.533	42.588	66.676	1.00	54.72	A	C
ATOM	5964	O	LEU	765	62.866	41.557	66.779	1.00	55.73	A	O
ATOM	5965	N	PRO	766	64.667	42.776	67.372	1.00	57.13	A	N
ATOM	5966	CD	PRO	766	65.545	43.960	67.317	1.00	57.88	A	C
ATOM	5967	CA	PRO	766	65.204	41.775	68.301	1.00	58.61	A	C
ATOM	5968	CB	PRO	766	66.600	42.309	68.604	1.00	58.49	A	C
ATOM	5969	CG	PRO	766	66.386	43.797	68.568	1.00	58.47	A	C
ATOM	5970	C	PRO	766	64.352	41.639	69.565	1.00	60.07	A	C
ATOM	5971	O	PRO	766	63.341	42.370	69.681	1.00	60.04	A	O
ATOM	5972	OXT	PRO	766	64.711	40.805	70.427	1.00	61.88	A	O
TER	5973		PRO	766						A	
ATOM	5974	CB	ASP	38	95.909	45.132	76.302	1.00	32.66	B	C
ATOM	5975	CG	ASP	38	96.954	46.047	75.698	1.00	32.61	B	C
ATOM	5976	OD1	ASP	38	96.905	47.269	75.977	1.00	30.88	B	O
ATOM	5977	OD2	ASP	38	97.816	45.544	74.942	1.00	31.65	B	O

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## FIG. 4 - 1 2 3

(Continued)

ATOM	5978	C	ASP	38	94.533	46.724	77.638	1.00	31.81	B	C
ATOM	5979	O	ASP	38	93.521	46.648	76.938	1.00	32.54	B	O
ATOM	5980	N	ASP	38	94.842	44.428	78.423	1.00	32.95	B	N
ATOM	5981	CA	ASP	38	95.507	45.557	77.717	1.00	32.06	B	C
ATOM	5982	N	SER	39	94.844	47.807	78.344	1.00	31.40	B	N
ATOM	5983	CA	SER	39	93.974	48.982	78.372	1.00	30.28	B	C
ATOM	5984	CB	SER	39	94.048	49.652	79.741	1.00	31.88	B	C
ATOM	5985	OG	SER	39	95.362	50.119	80.003	1.00	34.53	B	O
ATOM	5986	C	SER	39	94.289	50.017	77.305	1.00	29.15	B	C
ATOM	5987	O	SER	39	93.615	51.049	77.220	1.00	30.29	B	O
ATOM	5988	N	ARG	40	95.312	49.755	76.499	1.00	26.40	B	N
ATOM	5989	CA	ARG	40	95.685	50.686	75.442	1.00	24.29	B	C
ATOM	5990	CB	ARG	40	97.004	50.257	74.788	1.00	23.19	B	C
ATOM	5991	CG	ARG	40	98.228	50.429	75.670	1.00	20.84	B	C
ATOM	5992	CD	ARG	40	99.470	49.917	74.969	1.00	21.38	B	C
ATOM	5993	NE	ARG	40	99.404	48.479	74.728	1.00	21.28	B	N
ATOM	5994	CZ	ARG	40	100.260	47.812	73.963	1.00	22.73	B	C
ATOM	5995	NH1	ARG	40	101.247	48.461	73.361	1.00	22.52	B	N
ATOM	5996	NH2	ARG	40	100.134	46.497	73.806	1.00	22.23	B	N
ATOM	5997	C	ARG	40	94.604	50.757	74.376	1.00	23.29	B	C
ATOM	5998	O	ARG	40	93.881	49.793	74.150	1.00	23.24	B	O
ATOM	5999	N	LYS	41	94.494	51.907	73.725	1.00	23.55	B	N
ATOM	6000	CA	LYS	41	93.518	52.076	72.658	1.00	24.31	B	C
ATOM	6001	CB	LYS	41	93.386	53.556	72.274	1.00	25.29	B	C
ATOM	6002	CG	LYS	41	94.699	54.209	71.827	1.00	29.38	B	C
ATOM	6003	CD	LYS	41	94.505	55.663	71.365	1.00	28.84	B	C
ATOM	6004	CE	LYS	41	94.374	55.779	69.840	1.00	28.95	B	C
ATOM	6005	NZ	LYS	41	93.307	54.922	69.251	1.00	27.49	B	N
ATOM	6006	C	LYS	41	94.028	51.294	71.458	1.00	24.04	B	C
ATOM	6007	O	LYS	41	95.231	51.072	71.324	1.00	24.69	B	O
ATOM	6008	N	THR	42	93.118	50.859	70.595	1.00	23.54	B	N
ATOM	6009	CA	THR	42	93.518	50.130	69.399	1.00	22.29	B	C
ATOM	6010	CB	THR	42	92.454	49.083	68.959	1.00	22.69	B	C
ATOM	6011	OG1	THR	42	91.257	49.753	68.540	1.00	21.91	B	O
ATOM	6012	CG2	THR	42	92.128	48.129	70.101	1.00	20.28	B	C
ATOM	6013	C	THR	42	93.641	51.178	68.304	1.00	22.33	B	C
ATOM	6014	O	THR	42	93.386	52.363	68.541	1.00	23.36	B	O
ATOM	6015	N	TYR	43	94.045	50.750	67.116	1.00	20.55	B	N
ATOM	6016	CA	TYR	43	94.158	51.662	65.986	1.00	19.19	B	C
ATOM	6017	CB	TYR	43	95.233	51.153	65.020	1.00	20.32	B	C
ATOM	6018	CG	TYR	43	95.516	52.062	63.853	1.00	19.92	B	C
ATOM	6019	CD1	TYR	43	94.888	51.863	62.629	1.00	22.19	B	C
ATOM	6020	CE1	TYR	43	95.133	52.694	61.546	1.00	21.23	B	C
ATOM	6021	CD2	TYR	43	96.403	53.126	63.970	1.00	21.09	B	C
ATOM	6022	CE2	TYR	43	96.655	53.972	62.891	1.00	21.69	B	C
ATOM	6023	CZ	TYR	43	96.013	53.742	61.682	1.00	22.25	B	C
ATOM	6024	OH	TYR	43	96.247	54.553	60.600	1.00	25.44	B	O
ATOM	6025	C	TYR	43	92.770	51.631	65.349	1.00	18.52	B	C
ATOM	6026	O	TYR	43	92.396	50.640	64.725	1.00	17.41	B	O

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## FIG. 4 - 1 2 4

(Continued)

ATOM	6027	N	THR	44	92.007	52.709	65.532	1.00	17.70	B	N
ATOM	6028	CA	THR	44	90.633	52.802	65.019	1.00	18.55	B	C
ATOM	6029	CB	THR	44	89.762	53.748	65.877	1.00	16.45	B	C
ATOM	6030	OG1	THR	44	90.195	55.096	65.676	1.00	16.93	B	O
ATOM	6031	CG2	THR	44	89.875	53.409	67.346	1.00	14.45	B	C
ATOM	6032	C	THR	44	90.521	53.310	63.593	1.00	19.62	B	C
ATOM	6033	O	THR	44	91.511	53.741	62.992	1.00	21.89	B	O
ATOM	6034	N	LEU	45	89.296	53.277	63.067	1.00	19.06	B	N
ATOM	6035	CA	LEU	45	89.026	53.749	61.713	1.00	18.74	B	C
ATOM	6036	CB	LEU	45	87.570	53.489	61.327	1.00	17.33	B	C
ATOM	6037	CG	LEU	45	87.163	54.032	59.952	1.00	17.35	B	C
ATOM	6038	CD1	LEU	45	88.050	53.417	58.873	1.00	15.87	B	C
ATOM	6039	CD2	LEU	45	85.698	53.720	59.681	1.00	16.27	B	C
ATOM	6040	C	LEU	45	89.300	55.240	61.638	1.00	19.82	B	C
ATOM	6041	O	LEU	45	89.827	55.743	60.638	1.00	21.32	B	O
ATOM	6042	N	THR	46	88.948	55.945	62.707	1.00	19.07	B	N
ATOM	6043	CA	THR	46	89.156	57.382	62.760	1.00	20.55	B	C
ATOM	6044	CB	THR	46	88.550	57.988	64.038	1.00	21.32	B	C
ATOM	6045	OG1	THR	46	87.148	57.700	64.083	1.00	21.56	B	O
ATOM	6046	CG2	THR	46	88.745	59.497	64.053	1.00	20.61	B	C
ATOM	6047	C	THR	46	90.634	57.749	62.694	1.00	21.16	B	C
ATOM	6048	O	THR	46	90.999	58.759	62.092	1.00	21.06	B	O
ATOM	6049	N	ASP	47	91.491	56.945	63.313	1.00	21.00	B	N
ATOM	6050	CA	ASP	47	92.910	57.253	63.262	1.00	22.97	B	C
ATOM	6051	CB	ASP	47	93.731	56.273	64.110	1.00	25.34	B	C
ATOM	6052	CG	ASP	47	93.365	56.322	65.578	1.00	27.23	B	C
ATOM	6053	OD1	ASP	47	93.116	57.430	66.105	1.00	26.32	B	O
ATOM	6054	OD2	ASP	47	93.339	55.244	66.208	1.00	31.41	B	O
ATOM	6055	C	ASP	47	93.357	57.178	61.810	1.00	22.85	B	C
ATOM	6056	O	ASP	47	94.057	58.065	61.320	1.00	24.15	B	O
ATOM	6057	N	TYR	48	92.951	56.124	61.114	1.00	20.92	B	N
ATOM	6058	CA	TYR	48	93.332	55.998	59.720	1.00	21.40	B	C
ATOM	6059	CB	TYR	48	92.823	54.676	59.136	1.00	19.45	B	C
ATOM	6060	CG	TYR	48	92.867	54.612	57.624	1.00	18.60	B	C
ATOM	6061	CD1	TYR	48	94.062	54.787	56.927	1.00	18.00	B	C
ATOM	6062	CE1	TYR	48	94.098	54.734	55.531	1.00	16.57	B	C
ATOM	6063	CD2	TYR	48	91.702	54.383	56.885	1.00	21.30	B	C
ATOM	6064	CE2	TYR	48	91.726	54.329	55.489	1.00	19.50	B	C
ATOM	6065	CZ	TYR	48	92.925	54.503	54.822	1.00	18.43	B	C
ATOM	6066	OH	TYR	48	92.942	54.434	53.452	1.00	18.40	B	O
ATOM	6067	C	TYR	48	92.795	57.170	58.899	1.00	21.85	B	C
ATOM	6068	O	TYR	48	93.547	57.853	58.207	1.00	21.92	B	O
ATOM	6069	N	LEU	49	91.497	57.416	58.996	1.00	23.08	B	N
ATOM	6070	CA	LEU	49	90.885	58.485	58.223	1.00	26.78	B	C
ATOM	6071	CB	LEU	49	89.359	58.437	58.381	1.00	28.14	B	C
ATOM	6072	CG	LEU	49	88.688	57.157	57.872	1.00	28.75	B	C
ATOM	6073	CD1	LEU	49	87.188	57.305	57.980	1.00	28.04	B	C
ATOM	6074	CD2	LEU	49	89.094	56.889	56.420	1.00	28.45	B	C
ATOM	6075	C	LEU	49	91.391	59.886	58.544	1.00	28.33	B	C

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## FIG. 4 - 125

(Continued)

ATOM	6076	O	LEU	49	91.404	60.758	57.673	1.00	28.77	B	O
ATOM	6077	N	LYS	50	91.818	60.098	59.784	1.00	30.17	B	N
ATOM	6078	CA	LYS	50	92.299	61.407	60.204	1.00	30.95	B	C
ATOM	6079	CB	LYS	50	91.668	61.769	61.543	1.00	31.36	B	C
ATOM	6080	CG	LYS	50	90.159	61.743	61.478	1.00	33.25	B	C
ATOM	6081	CD	LYS	50	89.649	62.710	60.420	1.00	34.69	B	C
ATOM	6082	CE	LYS	50	88.239	62.353	59.970	1.00	36.08	B	C
ATOM	6083	NZ	LYS	50	87.310	62.113	61.113	1.00	37.00	B	N
ATOM	6084	C	LYS	50	93.811	61.543	60.288	1.00	31.05	B	C
ATOM	6085	O	LYS	50	94.325	62.622	60.577	1.00	32.05	B	O
ATOM	6086	N	ASN	51	94.525	60.456	60.033	1.00	30.75	B	N
ATOM	6087	CA	ASN	51	95.978	60.493	60.074	1.00	31.14	B	C
ATOM	6088	CB	ASN	51	96.502	61.541	59.090	1.00	33.97	B	C
ATOM	6089	CG	ASN	51	95.964	61.344	57.689	1.00	37.06	B	C
ATOM	6090	OD1	ASN	51	96.358	60.416	56.986	1.00	39.83	B	O
ATOM	6091	ND2	ASN	51	95.047	62.215	57.277	1.00	40.54	B	N
ATOM	6092	C	ASN	51	96.472	60.828	61.471	1.00	29.86	B	C
ATOM	6093	O	ASN	51	97.474	61.524	61.624	1.00	31.03	B	O
ATOM	6094	N	THR	52	95.770	60.335	62.486	1.00	27.96	B	N
ATOM	6095	CA	THR	52	96.152	60.587	63.870	1.00	26.81	B	C
ATOM	6096	CB	THR	52	95.315	59.742	64.854	1.00	27.15	B	C
ATOM	6097	OG1	THR	52	93.930	60.058	64.698	1.00	27.72	B	O
ATOM	6098	CG2	THR	52	95.724	60.030	66.291	1.00	25.06	B	C
ATOM	6099	C	THR	52	97.622	60.259	64.090	1.00	26.88	B	C
ATOM	6100	O	THR	52	98.274	60.867	64.934	1.00	27.07	B	O
ATOM	6101	N	TYR	53	98.141	59.298	63.328	1.00	26.35	B	N
ATOM	6102	CA	TYR	53	99.541	58.900	63.450	1.00	27.48	B	C
ATOM	6103	CB	TYR	53	99.632	57.446	63.899	1.00	24.69	B	C
ATOM	6104	CG	TYR	53	98.937	57.209	65.207	1.00	24.64	B	C
ATOM	6105	CD1	TYR	53	99.433	57.761	66.389	1.00	24.67	B	C
ATOM	6106	CE1	TYR	53	98.782	57.566	67.600	1.00	24.44	B	C
ATOM	6107	CD2	TYR	53	97.768	56.454	65.268	1.00	22.60	B	C
ATOM	6108	CE2	TYR	53	97.107	56.255	66.474	1.00	24.81	B	C
ATOM	6109	CZ	TYR	53	97.622	56.813	67.634	1.00	25.33	B	C
ATOM	6110	OH	TYR	53	96.981	56.609	68.826	1.00	25.74	B	O
ATOM	6111	C	TYR	53	100.279	59.076	62.131	1.00	29.01	B	C
ATOM	6112	O	TYR	53	100.187	58.234	61.239	1.00	30.80	B	O
ATOM	6113	N	ARG	54	101.024	60.168	62.019	1.00	30.00	B	N
ATOM	6114	CA	ARG	54	101.760	60.456	60.801	1.00	29.57	B	C
ATOM	6115	CB	ARG	54	101.718	61.955	60.498	1.00	32.42	B	C
ATOM	6116	CG	ARG	54	100.360	62.449	60.020	1.00	38.51	B	C
ATOM	6117	CD	ARG	54	100.364	63.945	59.724	1.00	42.89	B	C
ATOM	6118	NE	ARG	54	99.157	64.354	59.008	1.00	46.94	B	N
ATOM	6119	CZ	ARG	54	98.812	63.893	57.808	1.00	48.52	B	C
ATOM	6120	NH1	ARG	54	99.585	63.008	57.190	1.00	50.08	B	N
ATOM	6121	NH2	ARG	54	97.697	64.314	57.224	1.00	47.87	B	N
ATOM	6122	C	ARG	54	103.202	59.992	60.803	1.00	27.73	B	C
ATOM	6123	O	ARG	54	103.934	60.168	61.776	1.00	26.62	B	O
ATOM	6124	N	LEU	55	103.596	59.384	59.693	1.00	25.96	B	N

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## FIG. 4 - 1 2 6

(Continued)

ATOM	6125	CA	LEU	55	104.959	58.926	59.515	1.00	24.45	B	C
ATOM	6126	CB	LEU	55	105.025	57.911	58.382	1.00	22.51	B	C
ATOM	6127	CG	LEU	55	104.335	56.575	58.631	1.00	23.77	B	C
ATOM	6128	CD1	LEU	55	104.287	55.792	57.336	1.00	23.51	B	C
ATOM	6129	CD2	LEU	55	105.083	55.796	59.703	1.00	22.83	B	C
ATOM	6130	C	LEU	55	105.773	60.161	59.135	1.00	24.19	B	C
ATOM	6131	O	LEU	55	105.428	60.867	58.187	1.00	23.47	B	O
ATOM	6132	N	LYS	56	106.824	60.456	59.886	1.00	23.25	B	N
ATOM	6133	CA	LYS	56	107.631	61.603	59.532	1.00	23.81	B	C
ATOM	6134	CB	LYS	56	108.536	62.028	60.680	1.00	25.76	B	C
ATOM	6135	CG	LYS	56	107.850	62.922	61.697	1.00	29.15	B	C
ATOM	6136	CD	LYS	56	108.868	63.560	62.638	1.00	31.22	B	C
ATOM	6137	CE	LYS	56	108.225	64.593	63.548	1.00	32.59	B	C
ATOM	6138	NZ	LYS	56	109.235	65.233	64.439	1.00	34.54	B	N
ATOM	6139	C	LYS	56	108.458	61.196	58.330	1.00	23.35	B	C
ATOM	6140	O	LYS	56	108.833	60.035	58.186	1.00	23.24	B	O
ATOM	6141	N	LEU	57	108.717	62.162	57.462	1.00	22.99	B	N
ATOM	6142	CA	LEU	57	109.477	61.945	56.247	1.00	22.29	B	C
ATOM	6143	CB	LEU	57	108.612	62.292	55.040	1.00	23.21	B	C
ATOM	6144	CG	LEU	57	107.169	61.794	55.037	1.00	23.82	B	C
ATOM	6145	CD1	LEU	57	106.440	62.380	53.841	1.00	24.84	B	C
ATOM	6146	CD2	LEU	57	107.145	60.278	54.992	1.00	25.36	B	C
ATOM	6147	C	LEU	57	110.681	62.870	56.256	1.00	22.04	B	C
ATOM	6148	O	LEU	57	110.888	63.628	57.202	1.00	22.65	B	O
ATOM	6149	N	TYR	58	111.468	62.809	55.191	1.00	20.44	B	N
ATOM	6150	CA	TYR	58	112.624	63.674	55.065	1.00	20.14	B	C
ATOM	6151	CB	TYR	58	113.834	63.089	55.795	1.00	19.94	B	C
ATOM	6152	CG	TYR	58	114.933	64.099	56.008	1.00	18.95	B	C
ATOM	6153	CD1	TYR	58	115.845	64.392	54.998	1.00	19.13	B	C
ATOM	6154	CE1	TYR	58	116.816	65.380	55.165	1.00	18.92	B	C
ATOM	6155	CD2	TYR	58	115.022	64.816	57.201	1.00	19.88	B	C
ATOM	6156	CE2	TYR	58	115.987	65.807	57.378	1.00	19.69	B	C
ATOM	6157	CZ	TYR	58	116.877	66.086	56.355	1.00	19.43	B	C
ATOM	6158	OH	TYR	58	117.804	67.092	56.508	1.00	19.58	B	O
ATOM	6159	C	TYR	58	112.917	63.819	53.590	1.00	20.38	B	C
ATOM	6160	O	TYR	58	113.861	63.223	53.079	1.00	20.32	B	O
ATOM	6161	N	SER	59	112.085	64.604	52.909	1.00	21.33	B	N
ATOM	6162	CA	SER	59	112.245	64.839	51.479	1.00	22.11	B	C
ATOM	6163	CB	SER	59	110.920	65.275	50.852	1.00	21.08	B	C
ATOM	6164	OG	SER	59	109.985	64.212	50.843	1.00	24.94	B	O
ATOM	6165	C	SER	59	113.293	65.895	51.191	1.00	21.64	B	C
ATOM	6166	O	SER	59	113.099	67.064	51.491	1.00	23.87	B	O
ATOM	6167	N	LEU	60	114.404	65.485	50.602	1.00	21.76	B	N
ATOM	6168	CA	LEU	60	115.449	66.436	50.273	1.00	23.50	B	C
ATOM	6169	CB	LEU	60	116.752	66.062	50.986	1.00	22.27	B	C
ATOM	6170	CG	LEU	60	117.406	64.737	50.612	1.00	18.62	B	C
ATOM	6171	CD1	LEU	60	118.176	64.900	49.320	1.00	17.05	B	C
ATOM	6172	CD2	LEU	60	118.338	64.313	51.724	1.00	19.95	B	C
ATOM	6173	C	LEU	60	115.656	66.478	48.762	1.00	24.93	B	C

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(Continued)

## FIG. 4 - 1 2 7

ATOM	6174	O	LEU	60	115.176	65.604	48.029	1.00	23.79	B	O
ATOM	6175	N	ARG	61	116.375	67.495	48.302	1.00	26.02	B	N
ATOM	6176	CA	ARG	61	116.634	67.659	46.881	1.00	27.11	B	C
ATOM	6177	CB	ARG	61	115.693	68.728	46.329	1.00	32.13	B	C
ATOM	6178	CG	ARG	61	115.779	68.979	44.833	1.00	38.27	B	C
ATOM	6179	CD	ARG	61	115.002	70.243	44.495	1.00	41.78	B	C
ATOM	6180	NE	ARG	61	114.937	70.506	43.063	1.00	46.51	B	N
ATOM	6181	CZ	ARG	61	114.298	71.543	42.525	1.00	49.47	B	C
ATOM	6182	NH1	ARG	61	113.671	72.420	43.307	1.00	48.74	B	N
ATOM	6183	NH2	ARG	61	114.266	71.693	41.205	1.00	50.07	B	N
ATOM	6184	C	ARG	61	118.080	68.075	46.676	1.00	26.01	B	C
ATOM	6185	O	ARG	61	118.475	69.180	47.052	1.00	26.36	B	O
ATOM	6186	N	TRP	62	118.877	67.186	46.095	1.00	25.15	B	N
ATOM	6187	CA	TRP	62	120.282	67.488	45.846	1.00	24.48	B	C
ATOM	6188	CB	TRP	62	121.024	66.244	45.355	1.00	20.04	B	C
ATOM	6189	CG	TRP	62	121.095	65.145	46.365	1.00	18.16	B	C
ATOM	6190	CD2	TRP	62	121.954	65.092	47.508	1.00	14.54	B	C
ATOM	6191	CE2	TRP	62	121.639	63.910	48.215	1.00	15.18	B	C
ATOM	6192	CE3	TRP	62	122.956	65.932	48.007	1.00	12.41	B	C
ATOM	6193	CD1	TRP	62	120.315	64.017	46.419	1.00	17.39	B	C
ATOM	6194	NE1	TRP	62	120.639	63.272	47.528	1.00	15.77	B	N
ATOM	6195	CZ2	TRP	62	122.292	63.546	49.397	1.00	16.35	B	C
ATOM	6196	CZ3	TRP	62	123.606	65.575	49.183	1.00	14.94	B	C
ATOM	6197	CH2	TRP	62	123.271	64.389	49.866	1.00	16.25	B	C
ATOM	6198	C	TRP	62	120.401	68.588	44.798	1.00	26.73	B	C
ATOM	6199	O	TRP	62	119.863	68.457	43.698	1.00	27.86	B	O
ATOM	6200	N	ILE	63	121.088	69.675	45.135	1.00	27.97	B	N
ATOM	6201	CA	ILE	63	121.265	70.763	44.180	1.00	29.02	B	C
ATOM	6202	CB	ILE	63	120.947	72.130	44.803	1.00	29.64	B	C
ATOM	6203	CG2	ILE	63	119.476	72.193	45.169	1.00	30.36	B	C
ATOM	6204	CG1	ILE	63	121.830	72.372	46.027	1.00	30.01	B	C
ATOM	6205	CD1	ILE	63	121.542	73.682	46.736	1.00	27.88	B	C
ATOM	6206	C	ILE	63	122.693	70.771	43.657	1.00	30.19	B	C
ATOM	6207	O	ILE	63	123.062	71.609	42.835	1.00	31.12	B	O
ATOM	6208	N	SER	64	123.485	69.816	44.132	1.00	30.03	B	N
ATOM	6209	CA	SER	64	124.876	69.668	43.718	1.00	30.53	B	C
ATOM	6210	CB	SER	64	125.734	70.808	44.269	1.00	29.46	B	C
ATOM	6211	OG	SER	64	125.848	70.724	45.679	1.00	27.92	B	O
ATOM	6212	C	SER	64	125.399	68.343	44.255	1.00	31.08	B	C
ATOM	6213	O	SER	64	124.630	67.488	44.691	1.00	31.36	B	O
ATOM	6214	N	ASP	65	126.712	68.176	44.236	1.00	31.42	B	N
ATOM	6215	CA	ASP	65	127.306	66.947	44.728	1.00	32.55	B	C
ATOM	6216	CB	ASP	65	128.576	66.633	43.945	1.00	33.28	B	C
ATOM	6217	CG	ASP	65	129.158	65.286	44.302	1.00	35.12	B	C
ATOM	6218	OD1	ASP	65	128.446	64.261	44.158	1.00	33.02	B	O
ATOM	6219	OD2	ASP	65	130.331	65.259	44.728	1.00	37.02	B	O
ATOM	6220	C	ASP	65	127.636	67.045	46.211	1.00	32.66	B	C
ATOM	6221	O	ASP	65	128.076	66.069	46.818	1.00	31.78	B	O
ATOM	6222	N	HIS	66	127.399	68.217	46.796	1.00	33.06	B	N

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(Continued)

## FIG. 4 - 128

ATOM	6223	CA	HIS	66	127.704	68.440	48.203	1.00	32.64	B	C
ATOM	6224	CB	HIS	66	128.892	69.402	48.329	1.00	35.63	B	C
ATOM	6225	CG	HIS	66	130.032	69.076	47.416	1.00	39.09	B	C
ATOM	6226	CD2	HIS	66	131.260	68.562	47.669	1.00	40.29	B	C
ATOM	6227	ND1	HIS	66	129.959	69.238	46.047	1.00	41.80	B	N
ATOM	6228	CE1	HIS	66	131.092	68.835	45.498	1.00	42.37	B	C
ATOM	6229	NE2	HIS	66	131.897	68.420	46.459	1.00	42.11	B	N
ATOM	6230	C	HIS	66	126.547	69.001	49.016	1.00	31.01	B	C
ATOM	6231	O	HIS	66	126.602	69.008	50.245	1.00	30.92	B	O
ATOM	6232	N	GLU	67	125.505	69.479	48.345	1.00	30.05	B	N
ATOM	6233	CA	GLU	67	124.379	70.067	49.062	1.00	28.07	B	C
ATOM	6234	CB	GLU	67	124.457	71.591	48.984	1.00	27.21	B	C
ATOM	6235	CG	GLU	67	125.601	72.179	49.781	1.00	29.99	B	C
ATOM	6236	CD	GLU	67	125.745	73.675	49.593	1.00	32.09	B	C
ATOM	6237	OE1	GLU	67	126.408	74.315	50.438	1.00	33.25	B	O
ATOM	6238	OE2	GLU	67	125.207	74.209	48.599	1.00	34.83	B	O
ATOM	6239	C	GLU	67	123.015	69.619	48.583	1.00	27.52	B	C
ATOM	6240	O	GLU	67	122.872	69.085	47.482	1.00	27.10	B	O
ATOM	6241	N	TYR	68	122.012	69.855	49.425	1.00	26.72	B	N
ATOM	6242	CA	TYR	68	120.634	69.498	49.116	1.00	25.74	B	C
ATOM	6243	CB	TYR	68	120.347	68.069	49.592	1.00	23.47	B	C
ATOM	6244	CG	TYR	68	120.373	67.847	51.094	1.00	22.93	B	C
ATOM	6245	CD1	TYR	68	119.339	68.319	51.914	1.00	22.75	B	C
ATOM	6246	CE1	TYR	68	119.312	68.040	53.282	1.00	21.24	B	C
ATOM	6247	CD2	TYR	68	121.391	67.097	51.685	1.00	22.05	B	C
ATOM	6248	CE2	TYR	68	121.379	66.812	53.053	1.00	22.38	B	C
ATOM	6249	CZ	TYR	68	120.333	67.283	53.847	1.00	23.05	B	C
ATOM	6250	OH	TYR	68	120.300	66.973	55.191	1.00	18.34	B	O
ATOM	6251	C	TYR	68	119.657	70.481	49.759	1.00	26.00	B	C
ATOM	6252	O	TYR	68	119.961	71.077	50.789	1.00	26.50	B	O
ATOM	6253	N	LEU	69	118.497	70.674	49.139	1.00	26.72	B	N
ATOM	6254	CA	LEU	69	117.492	71.580	49.694	1.00	27.89	B	C
ATOM	6255	CB	LEU	69	116.729	72.316	48.586	1.00	24.29	B	C
ATOM	6256	CG	LEU	69	117.545	73.257	47.695	1.00	23.81	B	C
ATOM	6257	CD1	LEU	69	116.656	73.891	46.633	1.00	19.95	B	C
ATOM	6258	CD2	LEU	69	118.187	74.324	48.552	1.00	24.79	B	C
ATOM	6259	C	LEU	69	116.508	70.777	50.543	1.00	29.18	B	C
ATOM	6260	O	LEU	69	116.226	69.609	50.260	1.00	28.86	B	O
ATOM	6261	N	TYR	70	115.998	71.411	51.590	1.00	29.78	B	N
ATOM	6262	CA	TYR	70	115.057	70.765	52.482	1.00	31.48	B	C
ATOM	6263	CB	TYR	70	115.799	70.142	53.667	1.00	28.76	B	C
ATOM	6264	CG	TYR	70	114.910	69.348	54.592	1.00	26.47	B	C
ATOM	6265	CD1	TYR	70	114.396	68.114	54.206	1.00	25.75	B	C
ATOM	6266	CE1	TYR	70	113.544	67.398	55.038	1.00	26.40	B	C
ATOM	6267	CD2	TYR	70	114.553	69.847	55.842	1.00	28.33	B	C
ATOM	6268	CE2	TYR	70	113.701	69.141	56.686	1.00	28.03	B	C
ATOM	6269	CZ	TYR	70	113.199	67.918	56.276	1.00	28.21	B	C
ATOM	6270	OH	TYR	70	112.346	67.221	57.103	1.00	30.20	B	O
ATOM	6271	C	TYR	70	114.056	71.796	52.983	1.00	34.45	B	C

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## FIG. 4 - 129

(Continued)

ATOM	6272	O	TYR	70	114.425	72.914	53.336	1.00	33.43	B	O
ATOM	6273	N	LYS	71	112.787	71.410	53.002	1.00	39.59	B	N
ATOM	6274	CA	LYS	71	111.714	72.284	53.461	1.00	44.28	B	C
ATOM	6275	CB	LYS	71	110.408	71.904	52.763	1.00	45.57	B	C
ATOM	6276	CG	LYS	71	109.994	72.828	51.640	1.00	48.26	B	C
ATOM	6277	CD	LYS	71	109.416	74.116	52.192	1.00	51.24	B	C
ATOM	6278	CE	LYS	71	108.213	73.827	53.075	1.00	53.11	B	C
ATOM	6279	NZ	LYS	71	107.193	73.012	52.354	1.00	54.56	B	N
ATOM	6280	C	LYS	71	111.523	72.186	54.973	1.00	46.60	B	C
ATOM	6281	O	LYS	71	110.789	71.323	55.457	1.00	46.95	B	O
ATOM	6282	N	GLN	72	112.192	73.055	55.723	1.00	49.39	B	N
ATOM	6283	CA	GLN	72	112.040	73.042	57.172	1.00	52.01	B	C
ATOM	6284	CB	GLN	72	113.145	73.853	57.851	1.00	51.69	B	C
ATOM	6285	CG	GLN	72	113.126	73.763	59.373	1.00	52.37	B	C
ATOM	6286	CD	GLN	72	113.582	72.412	59.895	1.00	51.86	B	C
ATOM	6287	OE1	GLN	72	114.778	72.161	60.048	1.00	50.84	B	O
ATOM	6288	NE2	GLN	72	112.629	71.530	60.161	1.00	52.39	B	N
ATOM	6289	C	GLN	72	110.690	73.691	57.427	1.00	54.22	B	C
ATOM	6290	O	GLN	72	109.890	73.814	56.498	1.00	54.44	B	O
ATOM	6291	N	GLU	73	110.447	74.100	58.672	1.00	56.57	B	N
ATOM	6292	CA	GLU	73	109.197	74.745	59.075	1.00	58.47	B	C
ATOM	6293	CB	GLU	73	109.498	76.089	59.738	1.00	60.20	B	C
ATOM	6294	CG	GLU	73	110.530	76.022	60.861	1.00	62.04	B	C
ATOM	6295	CD	GLU	73	110.065	75.206	62.055	1.00	62.79	B	C
ATOM	6296	OE1	GLU	73	110.815	75.145	63.053	1.00	64.53	B	O
ATOM	6297	OE2	GLU	73	108.957	74.628	62.001	1.00	62.71	B	O
ATOM	6298	C	GLU	73	108.293	74.962	57.867	1.00	59.40	B	C
ATOM	6299	O	GLU	73	107.242	74.329	57.733	1.00	61.08	B	O
ATOM	6300	N	ASN	74	108.717	75.863	56.989	1.00	58.30	B	N
ATOM	6301	CA	ASN	74	107.987	76.156	55.768	1.00	57.33	B	C
ATOM	6302	CB	ASN	74	106.771	77.035	56.054	1.00	59.07	B	C
ATOM	6303	CG	ASN	74	105.474	76.399	55.581	1.00	60.80	B	C
ATOM	6304	OD1	ASN	74	105.350	76.006	54.418	1.00	61.62	B	O
ATOM	6305	ND2	ASN	74	104.501	76.293	56.482	1.00	60.69	B	N
ATOM	6306	C	ASN	74	108.938	76.858	54.815	1.00	56.35	B	C
ATOM	6307	O	ASN	74	108.666	76.979	53.620	1.00	56.72	B	O
ATOM	6308	N	ASN	75	110.059	77.321	55.355	1.00	54.35	B	N
ATOM	6309	CA	ASN	75	111.064	77.984	54.544	1.00	52.33	B	C
ATOM	6310	CB	ASN	75	111.793	79.055	55.355	1.00	55.77	B	C
ATOM	6311	CG	ASN	75	111.992	78.659	56.793	1.00	57.61	B	C
ATOM	6312	OD1	ASN	75	112.467	77.563	57.088	1.00	60.07	B	O
ATOM	6313	ND2	ASN	75	111.635	79.556	57.705	1.00	59.51	B	N
ATOM	6314	C	ASN	75	112.048	76.943	54.026	1.00	49.25	B	C
ATOM	6315	O	ASN	75	112.052	75.798	54.477	1.00	49.19	B	O
ATOM	6316	N	ILE	76	112.883	77.343	53.077	1.00	45.23	B	N
ATOM	6317	CA	ILE	76	113.837	76.424	52.483	1.00	41.55	B	C
ATOM	6318	CB	ILE	76	113.871	76.616	50.962	1.00	41.68	B	C
ATOM	6319	CG2	ILE	76	114.705	75.524	50.310	1.00	41.39	B	C
ATOM	6320	CG1	ILE	76	112.445	76.583	50.415	1.00	40.24	B	C

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(Continued)

## FIG. 4 - 130

ATOM	6321	CD1	ILE	76	112.341	77.009	48.967	1.00	42.01	B	C
ATOM	6322	C	ILE	76	115.243	76.589	53.043	1.00	39.85	B	C
ATOM	6323	O	ILE	76	115.758	77.701	53.150	1.00	41.15	B	O
ATOM	6324	N	LEU	77	115.862	75.472	53.400	1.00	36.42	B	N
ATOM	6325	CA	LEU	77	117.208	75.498	53.941	1.00	34.22	B	C
ATOM	6326	CB	LEU	77	117.227	74.901	55.351	1.00	34.28	B	C
ATOM	6327	CG	LEU	77	116.155	75.359	56.346	1.00	34.54	B	C
ATOM	6328	CD1	LEU	77	116.435	74.728	57.701	1.00	33.23	B	C
ATOM	6329	CD2	LEU	77	116.149	76.874	56.460	1.00	34.45	B	C
ATOM	6330	C	LEU	77	118.121	74.683	53.036	1.00	32.91	B	C
ATOM	6331	O	LEU	77	117.657	73.821	52.289	1.00	32.49	B	O
ATOM	6332	N	VAL	78	119.417	74.967	53.103	1.00	30.72	B	N
ATOM	6333	CA	VAL	78	120.409	74.253	52.308	1.00	29.87	B	C
ATOM	6334	CB	VAL	78	121.227	75.227	51.431	1.00	30.20	B	C
ATOM	6335	CG1	VAL	78	122.327	74.480	50.691	1.00	29.01	B	C
ATOM	6336	CG2	VAL	78	120.311	75.906	50.448	1.00	31.37	B	C
ATOM	6337	C	VAL	78	121.346	73.523	53.263	1.00	28.37	B	C
ATOM	6338	O	VAL	78	121.781	74.087	54.261	1.00	28.38	B	O
ATOM	6339	N	PHE	79	121.660	72.272	52.956	1.00	26.51	B	N
ATOM	6340	CA	PHE	79	122.530	71.496	53.821	1.00	24.85	B	C
ATOM	6341	CB	PHE	79	121.807	70.247	54.338	1.00	24.45	B	C
ATOM	6342	CG	PHE	79	120.680	70.531	55.296	1.00	22.62	B	C
ATOM	6343	CD1	PHE	79	119.499	71.120	54.857	1.00	20.15	B	C
ATOM	6344	CD2	PHE	79	120.789	70.168	56.636	1.00	19.84	B	C
ATOM	6345	CE1	PHE	79	118.448	71.338	55.733	1.00	20.35	B	C
ATOM	6346	CE2	PHE	79	119.749	70.382	57.513	1.00	16.96	B	C
ATOM	6347	CZ	PHE	79	118.573	70.967	57.065	1.00	18.97	B	C
ATOM	6348	C	PHE	79	123.815	71.036	53.151	1.00	24.95	B	C
ATOM	6349	O	PHE	79	123.841	70.729	51.960	1.00	24.94	B	O
ATOM	6350	N	ASN	80	124.876	70.992	53.948	1.00	23.66	B	N
ATOM	6351	CA	ASN	80	126.174	70.518	53.517	1.00	23.32	B	C
ATOM	6352	CB	ASN	80	127.276	71.307	54.220	1.00	22.91	B	C
ATOM	6353	CG	ASN	80	128.653	70.689	54.032	1.00	22.91	B	C
ATOM	6354	OD1	ASN	80	128.916	69.567	54.486	1.00	23.26	B	O
ATOM	6355	ND2	ASN	80	129.542	71.421	53.364	1.00	21.99	B	N
ATOM	6356	C	ASN	80	126.156	69.077	54.018	1.00	24.17	B	C
ATOM	6357	O	ASN	80	126.168	68.842	55.222	1.00	25.80	B	O
ATOM	6358	N	ALA	81	126.116	68.116	53.105	1.00	23.17	B	N
ATOM	6359	CA	ALA	81	126.054	66.713	53.496	1.00	24.07	B	C
ATOM	6360	CB	ALA	81	126.025	65.819	52.246	1.00	20.69	B	C
ATOM	6361	C	ALA	81	127.167	66.256	54.434	1.00	25.23	B	C
ATOM	6362	O	ALA	81	126.925	65.462	55.347	1.00	25.26	B	O
ATOM	6363	N	GLU	82	128.377	66.764	54.222	1.00	26.73	B	N
ATOM	6364	CA	GLU	82	129.525	66.351	55.024	1.00	29.51	B	C
ATOM	6365	CB	GLU	82	130.820	66.835	54.361	1.00	32.02	B	C
ATOM	6366	CG	GLU	82	132.124	66.326	55.005	1.00	35.72	B	C
ATOM	6367	CD	GLU	82	132.287	64.800	54.955	1.00	38.90	B	C
ATOM	6368	OE1	GLU	82	132.064	64.191	53.884	1.00	38.71	B	O
ATOM	6369	OE2	GLU	82	132.659	64.209	55.995	1.00	40.81	B	O

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## FIG. 4 - 131

(Continued)

ATOM	6370	C	GLU	82	129.528	66.757	56.497	1.00	29.17	B	C
ATOM	6371	O	GLU	82	130.102	66.051	57.324	1.00	28.55	B	O
ATOM	6372	N	TYR	83	128.888	67.872	56.834	1.00	29.07	B	N
ATOM	6373	CA	TYR	83	128.877	68.329	58.223	1.00	28.95	B	C
ATOM	6374	CB	TYR	83	129.504	69.722	58.320	1.00	30.17	B	C
ATOM	6375	CG	TYR	83	130.821	69.834	57.596	1.00	33.40	B	C
ATOM	6376	CD1	TYR	83	131.914	69.049	57.963	1.00	33.79	B	C
ATOM	6377	CE1	TYR	83	133.120	69.129	57.271	1.00	36.07	B	C
ATOM	6378	CD2	TYR	83	130.966	70.704	56.517	1.00	35.97	B	C
ATOM	6379	CE2	TYR	83	132.162	70.791	55.815	1.00	36.91	B	C
ATOM	6380	CZ	TYR	83	133.234	70.003	56.195	1.00	38.12	B	C
ATOM	6381	OH	TYR	83	134.413	70.091	55.486	1.00	42.42	B	O
ATOM	6382	C	TYR	83	127.490	68.355	58.853	1.00	28.16	B	C
ATOM	6383	O	TYR	83	127.340	68.093	60.044	1.00	29.04	B	O
ATOM	6384	N	GLY	84	126.478	68.684	58.063	1.00	25.68	B	N
ATOM	6385	CA	GLY	84	125.136	68.726	58.601	1.00	24.77	B	C
ATOM	6386	C	GLY	84	124.668	70.137	58.880	1.00	24.95	B	C
ATOM	6387	O	GLY	84	123.511	70.345	59.222	1.00	23.68	B	O
ATOM	6388	N	ASN	85	125.565	71.109	58.745	1.00	26.40	B	N
ATOM	6389	CA	ASN	85	125.201	72.501	58.984	1.00	27.79	B	C
ATOM	6390	CB	ASN	85	126.446	73.366	59.181	1.00	28.01	B	C
ATOM	6391	CG	ASN	85	127.356	73.363	57.975	1.00	31.32	B	C
ATOM	6392	OD1	ASN	85	128.051	72.384	57.697	1.00	31.73	B	O
ATOM	6393	ND2	ASN	85	127.338	74.472	57.250	1.00	33.71	B	N
ATOM	6394	C	ASN	85	124.381	73.023	57.813	1.00	28.62	B	C
ATOM	6395	O	ASN	85	124.432	72.472	56.720	1.00	28.74	B	O
ATOM	6396	N	SER	86	123.622	74.085	58.043	1.00	30.17	B	N
ATOM	6397	CA	SER	86	122.787	74.633	56.991	1.00	32.38	B	C
ATOM	6398	CB	SER	86	121.392	74.005	57.061	1.00	31.71	B	C
ATOM	6399	OG	SER	86	120.734	74.380	58.256	1.00	32.32	B	O
ATOM	6400	C	SER	86	122.658	76.145	57.063	1.00	33.63	B	C
ATOM	6401	O	SER	86	123.307	76.800	57.874	1.00	34.72	B	O
ATOM	6402	N	SER	87	121.806	76.682	56.195	1.00	35.45	B	N
ATOM	6403	CA	SER	87	121.530	78.111	56.115	1.00	35.95	B	C
ATOM	6404	CB	SER	87	122.588	78.825	55.280	1.00	35.50	B	C
ATOM	6405	OG	SER	87	123.887	78.635	55.810	1.00	39.27	B	O
ATOM	6406	C	SER	87	120.191	78.233	55.418	1.00	36.74	B	C
ATOM	6407	O	SER	87	119.832	77.369	54.625	1.00	38.47	B	O
ATOM	6408	N	VAL	88	119.444	79.288	55.723	1.00	37.17	B	N
ATOM	6409	CA	VAL	88	118.154	79.498	55.084	1.00	36.32	B	C
ATOM	6410	CB	VAL	88	117.357	80.636	55.750	1.00	37.21	B	C
ATOM	6411	CG1	VAL	88	116.094	80.916	54.954	1.00	36.84	B	C
ATOM	6412	CG2	VAL	88	117.006	80.260	57.186	1.00	38.04	B	C
ATOM	6413	C	VAL	88	118.422	79.897	53.647	1.00	36.83	B	C
ATOM	6414	O	VAL	88	119.235	80.782	53.379	1.00	36.34	B	O
ATOM	6415	N	PHE	89	117.745	79.240	52.719	1.00	36.53	B	N
ATOM	6416	CA	PHE	89	117.925	79.552	51.314	1.00	37.05	B	C
ATOM	6417	CB	PHE	89	117.901	78.262	50.491	1.00	34.62	B	C
ATOM	6418	CG	PHE	89	118.060	78.474	49.014	1.00	31.67	B	C

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## FIG. 4 - 132

(Continued)

ATOM	6419	CD1	PHE	89	116.963	78.790	48.223	1.00	29.04	B	C
ATOM	6420	CD2	PHE	89	119.303	78.333	48.412	1.00	31.62	B	C
ATOM	6421	CE1	PHE	89	117.095	78.958	46.857	1.00	28.72	B	C
ATOM	6422	CE2	PHE	89	119.450	78.500	47.038	1.00	32.27	B	C
ATOM	6423	CZ	PHE	89	118.342	78.813	46.258	1.00	30.91	B	C
ATOM	6424	C	PHE	89	116.801	80.483	50.896	1.00	39.38	B	C
ATOM	6425	O	PHE	89	116.901	81.188	49.892	1.00	39.89	B	O
ATOM	6426	N	LEU	90	115.733	80.493	51.688	1.00	41.53	B	N
ATOM	6427	CA	LEU	90	114.581	81.332	51.403	1.00	43.78	B	C
ATOM	6428	CB	LEU	90	113.849	80.788	50.173	1.00	44.69	B	C
ATOM	6429	CG	LEU	90	112.818	81.664	49.462	1.00	44.94	B	C
ATOM	6430	CD1	LEU	90	113.439	83.000	49.088	1.00	44.39	B	C
ATOM	6431	CD2	LEU	90	112.328	80.944	48.217	1.00	44.54	B	C
ATOM	6432	C	LEU	90	113.653	81.348	52.613	1.00	45.79	B	C
ATOM	6433	O	LEU	90	113.192	80.302	53.062	1.00	44.77	B	O
ATOM	6434	N	GLU	91	113.395	82.542	53.140	1.00	49.59	B	N
ATOM	6435	CA	GLU	91	112.524	82.715	54.302	1.00	51.78	B	C
ATOM	6436	CB	GLU	91	112.571	84.166	54.790	1.00	53.90	B	C
ATOM	6437	CG	GLU	91	113.950	84.663	55.199	1.00	58.64	B	C
ATOM	6438	CD	GLU	91	114.432	84.070	56.511	1.00	61.93	B	C
ATOM	6439	OE1	GLU	91	114.607	82.835	56.585	1.00	64.17	B	O
ATOM	6440	OE2	GLU	91	114.639	84.843	57.472	1.00	63.53	B	O
ATOM	6441	C	GLU	91	111.083	82.352	53.961	1.00	52.17	B	C
ATOM	6442	O	GLU	91	110.549	82.777	52.939	1.00	50.91	B	O
ATOM	6443	N	ASN	92	110.452	81.576	54.835	1.00	53.63	B	N
ATOM	6444	CA	ASN	92	109.073	81.146	54.631	1.00	54.46	B	C
ATOM	6445	CB	ASN	92	108.654	80.205	55.761	1.00	55.64	B	C
ATOM	6446	CG	ASN	92	108.451	80.934	57.074	1.00	57.59	B	C
ATOM	6447	OD1	ASN	92	109.140	81.914	57.362	1.00	59.33	B	O
ATOM	6448	ND2	ASN	92	107.512	80.451	57.885	1.00	57.67	B	N
ATOM	6449	C	ASN	92	108.116	82.336	54.581	1.00	53.80	B	C
ATOM	6450	O	ASN	92	106.924	82.171	54.328	1.00	53.09	B	O
ATOM	6451	N	SER	93	108.646	83.532	54.818	1.00	53.62	B	N
ATOM	6452	CA	SER	93	107.833	84.744	54.813	1.00	53.91	B	C
ATOM	6453	CB	SER	93	108.078	85.527	56.100	1.00	53.85	B	C
ATOM	6454	OG	SER	93	109.438	85.905	56.196	1.00	54.56	B	O
ATOM	6455	C	SER	93	108.097	85.658	53.618	1.00	53.82	B	C
ATOM	6456	O	SER	93	107.391	86.646	53.421	1.00	52.94	B	O
ATOM	6457	N	THR	94	109.107	85.322	52.819	1.00	54.56	B	N
ATOM	6458	CA	THR	94	109.473	86.127	51.656	1.00	54.56	B	C
ATOM	6459	CB	THR	94	110.616	85.473	50.858	1.00	54.40	B	C
ATOM	6460	OG1	THR	94	110.837	86.210	49.648	1.00	53.65	B	O
ATOM	6461	CG2	THR	94	110.268	84.040	50.515	1.00	55.54	B	C
ATOM	6462	C	THR	94	108.330	86.418	50.689	1.00	54.94	B	C
ATOM	6463	O	THR	94	108.424	87.339	49.878	1.00	55.42	B	O
ATOM	6464	N	PHE	95	107.256	85.640	50.762	1.00	54.35	B	N
ATOM	6465	CA	PHE	95	106.125	85.865	49.873	1.00	54.57	B	C
ATOM	6466	CB	PHE	95	105.956	84.681	48.914	1.00	53.35	B	C
ATOM	6467	CG	PHE	95	107.158	84.426	48.043	1.00	52.21	B	C

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(Continued)

## FIG. 4 - 133

ATOM	6468	CD1 PHE	95	107.978	83.326	48.268	1.00	51.86	B	C
ATOM	6469	CD2 PHE	95	107.476	85.290	47.005	1.00	51.89	B	C
ATOM	6470	CE1 PHE	95	109.095	83.091	47.473	1.00	50.37	B	C
ATOM	6471	CE2 PHE	95	108.594	85.061	46.205	1.00	51.43	B	C
ATOM	6472	CZ PHE	95	109.403	83.960	46.441	1.00	50.62	B	C
ATOM	6473	C PHE	95	104.825	86.105	50.639	1.00	55.66	B	C
ATOM	6474	O PHE	95	103.740	85.784	50.149	1.00	55.16	B	O
ATOM	6475	N ASP	96	104.941	86.681	51.835	1.00	56.69	B	N
ATOM	6476	CA ASP	96	103.775	86.964	52.668	1.00	57.24	B	C
ATOM	6477	CB ASP	96	104.167	87.785	53.900	1.00	58.96	B	C
ATOM	6478	CG ASP	96	104.793	86.945	54.993	1.00	60.91	B	C
ATOM	6479	OD1 ASP	96	104.234	85.875	55.321	1.00	60.82	B	O
ATOM	6480	OD2 ASP	96	105.835	87.366	55.538	1.00	62.59	B	O
ATOM	6481	C ASP	96	102.674	87.712	51.933	1.00	57.24	B	C
ATOM	6482	O ASP	96	101.498	87.401	52.100	1.00	58.26	B	O
ATOM	6483	N GLU	97	103.050	88.703	51.130	1.00	57.07	B	N
ATOM	6484	CA GLU	97	102.068	89.496	50.395	1.00	57.68	B	C
ATOM	6485	CB GLU	97	102.389	90.994	50.512	1.00	59.15	B	C
ATOM	6486	CG GLU	97	102.397	91.553	51.935	1.00	61.76	B	C
ATOM	6487	CD GLU	97	103.629	91.140	52.729	1.00	63.57	B	C
ATOM	6488	OE1 GLU	97	103.714	91.490	53.927	1.00	63.88	B	O
ATOM	6489	OE2 GLU	97	104.514	90.467	52.155	1.00	64.73	B	O
ATOM	6490	C GLU	97	101.970	89.123	48.917	1.00	56.86	B	C
ATOM	6491	O GLU	97	101.652	89.972	48.080	1.00	58.05	B	O
ATOM	6492	N PHE	98	102.234	87.859	48.598	1.00	54.75	B	N
ATOM	6493	CA PHE	98	102.181	87.393	47.214	1.00	52.58	B	C
ATOM	6494	CB PHE	98	102.730	85.965	47.117	1.00	52.53	B	C
ATOM	6495	CG PHE	98	102.792	85.434	45.713	1.00	51.74	B	C
ATOM	6496	CD1 PHE	98	103.564	86.073	44.749	1.00	50.75	B	C
ATOM	6497	CD2 PHE	98	102.064	84.305	45.348	1.00	51.54	B	C
ATOM	6498	CE1 PHE	98	103.609	85.597	43.445	1.00	50.51	B	C
ATOM	6499	CE2 PHE	98	102.103	83.822	44.044	1.00	50.40	B	C
ATOM	6500	CZ PHE	98	102.876	84.469	43.092	1.00	49.83	B	C
ATOM	6501	C PHE	98	100.764	87.448	46.641	1.00	51.24	B	C
ATOM	6502	O PHE	98	100.578	87.544	45.427	1.00	50.42	B	O
ATOM	6503	N GLY	99	99.770	87.383	47.523	1.00	50.67	B	N
ATOM	6504	CA GLY	99	98.383	87.441	47.094	1.00	48.74	B	C
ATOM	6505	C GLY	99	97.918	86.192	46.376	1.00	47.41	B	C
ATOM	6506	O GLY	99	97.020	86.246	45.540	1.00	48.42	B	O
ATOM	6507	N HIS	100	98.530	85.065	46.712	1.00	45.49	B	N
ATOM	6508	CA HIS	100	98.200	83.780	46.104	1.00	43.24	B	C
ATOM	6509	CB HIS	100	98.787	83.686	44.694	1.00	41.93	B	C
ATOM	6510	CG HIS	100	98.004	84.414	43.651	1.00	39.37	B	C
ATOM	6511	CD2 HIS	100	98.345	85.437	42.833	1.00	38.83	B	C
ATOM	6512	ND1 HIS	100	96.711	84.075	43.321	1.00	39.65	B	N
ATOM	6513	CE1 HIS	100	96.288	84.857	42.344	1.00	38.90	B	C
ATOM	6514	NE2 HIS	100	97.262	85.691	42.029	1.00	38.71	B	N
ATOM	6515	C HIS	100	98.822	82.677	46.940	1.00	42.56	B	C
ATOM	6516	O HIS	100	99.916	82.846	47.473	1.00	43.12	B	O

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## FIG. 4 - 134

(Continued)

ATOM	6517	N	SER	101	98.139	81.547	47.063	1.00	41.90	B	N
ATOM	6518	CA	SER	101	98.716	80.442	47.817	1.00	43.20	B	C
ATOM	6519	CB	SER	101	97.623	79.527	48.382	1.00	43.41	B	C
ATOM	6520	OG	SER	101	96.852	78.931	47.354	1.00	44.00	B	O
ATOM	6521	C	SER	101	99.582	79.680	46.820	1.00	42.92	B	C
ATOM	6522	O	SER	101	99.083	79.213	45.794	1.00	43.33	B	O
ATOM	6523	N	ILE	102	100.880	79.584	47.095	1.00	41.90	B	N
ATOM	6524	CA	ILE	102	101.762	78.874	46.183	1.00	42.10	B	C
ATOM	6525	CB	ILE	102	103.255	79.286	46.369	1.00	43.10	B	C
ATOM	6526	CG2	ILE	102	103.370	80.811	46.404	1.00	43.52	B	C
ATOM	6527	CG1	ILE	102	103.824	78.700	47.660	1.00	45.01	B	C
ATOM	6528	CD1	ILE	102	105.294	79.038	47.895	1.00	46.96	B	C
ATOM	6529	C	ILE	102	101.598	77.380	46.415	1.00	41.08	B	C
ATOM	6530	O	ILE	102	101.677	76.901	47.544	1.00	41.27	B	O
ATOM	6531	N	ASN	103	101.342	76.648	45.339	1.00	40.05	B	N
ATOM	6532	CA	ASN	103	101.157	75.211	45.434	1.00	39.20	B	C
ATOM	6533	CB	ASN	103	100.502	74.674	44.163	1.00	39.98	B	C
ATOM	6534	CG	ASN	103	100.190	73.199	44.257	1.00	39.82	B	C
ATOM	6535	OD1	ASN	103	99.355	72.784	45.056	1.00	40.83	B	O
ATOM	6536	ND2	ASN	103	100.866	72.396	43.448	1.00	40.75	B	N
ATOM	6537	C	ASN	103	102.486	74.508	45.645	1.00	37.42	B	C
ATOM	6538	O	ASN	103	102.601	73.614	46.475	1.00	38.46	B	O
ATOM	6539	N	ASP	104	103.491	74.912	44.880	1.00	35.77	B	N
ATOM	6540	CA	ASP	104	104.808	74.303	44.982	1.00	34.14	B	C
ATOM	6541	CB	ASP	104	104.819	72.955	44.248	1.00	33.54	B	C
ATOM	6542	CG	ASP	104	105.987	72.072	44.655	1.00	34.77	B	C
ATOM	6543	OD1	ASP	104	106.061	70.919	44.178	1.00	33.72	B	O
ATOM	6544	OD2	ASP	104	106.835	72.525	45.453	1.00	35.84	B	O
ATOM	6545	C	ASP	104	105.827	75.253	44.367	1.00	33.07	B	C
ATOM	6546	O	ASP	104	105.461	76.218	43.695	1.00	33.54	B	O
ATOM	6547	N	TYR	105	107.103	74.985	44.607	1.00	32.32	B	N
ATOM	6548	CA	TYR	105	108.167	75.824	44.082	1.00	31.45	B	C
ATOM	6549	CB	TYR	105	108.854	76.573	45.220	1.00	32.58	B	C
ATOM	6550	CG	TYR	105	109.515	75.662	46.218	1.00	35.82	B	C
ATOM	6551	CD1	TYR	105	110.859	75.306	46.091	1.00	36.01	B	C
ATOM	6552	CE1	TYR	105	111.465	74.453	47.009	1.00	36.30	B	C
ATOM	6553	CD2	TYR	105	108.791	75.138	47.287	1.00	37.55	B	C
ATOM	6554	CE2	TYR	105	109.387	74.282	48.208	1.00	38.47	B	C
ATOM	6555	CZ	TYR	105	110.719	73.947	48.065	1.00	37.17	B	C
ATOM	6556	OH	TYR	105	111.293	73.106	48.984	1.00	38.67	B	O
ATOM	6557	C	TYR	105	109.180	74.972	43.347	1.00	30.07	B	C
ATOM	6558	O	TYR	105	109.048	73.754	43.276	1.00	29.32	B	O
ATOM	6559	N	SER	106	110.203	75.623	42.815	1.00	28.45	B	N
ATOM	6560	CA	SER	106	111.236	74.938	42.059	1.00	26.63	B	C
ATOM	6561	CB	SER	106	110.648	74.391	40.758	1.00	24.49	B	C
ATOM	6562	OG	SER	106	111.662	74.145	39.806	1.00	24.16	B	O
ATOM	6563	C	SER	106	112.341	75.926	41.745	1.00	26.32	B	C
ATOM	6564	O	SER	106	112.168	76.821	40.919	1.00	28.04	B	O
ATOM	6565	N	ILE	107	113.475	75.770	42.413	1.00	25.01	B	N

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## FIG. 4 - 135

(Continued)

ATOM	6566	CA	ILE	107	114.602	76.662	42.196	1.00	24.30	B	C
ATOM	6567	CB	ILE	107	115.634	76.576	43.354	1.00	21.79	B	C
ATOM	6568	CG2	ILE	107	116.885	77.328	42.987	1.00	21.05	B	C
ATOM	6569	CG1	ILE	107	115.050	77.161	44.639	1.00	21.30	B	C
ATOM	6570	CD1	ILE	107	114.056	76.271	45.321	1.00	23.96	B	C
ATOM	6571	C	ILE	107	115.315	76.305	40.901	1.00	25.00	B	C
ATOM	6572	O	ILE	107	115.418	75.132	40.548	1.00	27.32	B	O
ATOM	6573	N	SER	108	115.788	77.320	40.187	1.00	24.67	B	N
ATOM	6574	CA	SER	108	116.534	77.102	38.959	1.00	24.23	B	C
ATOM	6575	CB	SER	108	116.936	78.439	38.350	1.00	23.85	B	C
ATOM	6576	OG	SER	108	117.786	79.144	39.245	1.00	23.56	B	O
ATOM	6577	C	SER	108	117.789	76.347	39.403	1.00	25.01	B	C
ATOM	6578	O	SER	108	118.223	76.484	40.546	1.00	25.28	B	O
ATOM	6579	N	PRO	109	118.394	75.554	38.508	1.00	25.25	B	N
ATOM	6580	CD	PRO	109	118.003	75.282	37.115	1.00	25.10	B	C
ATOM	6581	CA	PRO	109	119.600	74.798	38.869	1.00	26.01	B	C
ATOM	6582	CB	PRO	109	120.023	74.172	37.547	1.00	24.74	B	C
ATOM	6583	CG	PRO	109	118.722	73.983	36.836	1.00	25.99	B	C
ATOM	6584	C	PRO	109	120.726	75.619	39.499	1.00	27.62	B	C
ATOM	6585	O	PRO	109	121.413	75.139	40.403	1.00	28.26	B	O
ATOM	6586	N	ASP	110	120.923	76.847	39.026	1.00	28.44	B	N
ATOM	6587	CA	ASP	110	121.988	77.691	39.562	1.00	29.86	B	C
ATOM	6588	CB	ASP	110	122.465	78.689	38.504	1.00	30.74	B	C
ATOM	6589	CG	ASP	110	121.342	79.543	37.960	1.00	32.54	B	C
ATOM	6590	OD1	ASP	110	120.415	79.856	38.730	1.00	33.07	B	O
ATOM	6591	OD2	ASP	110	121.391	79.912	36.767	1.00	33.02	B	O
ATOM	6592	C	ASP	110	121.599	78.449	40.828	1.00	30.83	B	C
ATOM	6593	O	ASP	110	122.379	79.248	41.337	1.00	32.09	B	O
ATOM	6594	N	GLY	111	120.397	78.197	41.335	1.00	31.58	B	N
ATOM	6595	CA	GLY	111	119.945	78.863	42.545	1.00	32.15	B	C
ATOM	6596	C	GLY	111	119.673	80.343	42.357	1.00	32.90	B	C
ATOM	6597	O	GLY	111	119.462	81.074	43.323	1.00	31.87	B	O
ATOM	6598	N	GLN	112	119.666	80.783	41.105	1.00	33.93	B	N
ATOM	6599	CA	GLN	112	119.440	82.184	40.783	1.00	35.14	B	C
ATOM	6600	CB	GLN	112	120.005	82.486	39.396	1.00	36.07	B	C
ATOM	6601	CG	GLN	112	120.885	83.717	39.329	1.00	39.16	B	C
ATOM	6602	CD	GLN	112	122.019	83.551	38.337	1.00	39.62	B	C
ATOM	6603	OE1	GLN	112	122.890	82.697	38.515	1.00	38.31	B	O
ATOM	6604	NE2	GLN	112	122.013	84.363	37.281	1.00	41.28	B	N
ATOM	6605	C	GLN	112	117.970	82.577	40.826	1.00	34.39	B	C
ATOM	6606	O	GLN	112	117.627	83.692	41.225	1.00	35.13	B	O
ATOM	6607	N	PHE	113	117.099	81.667	40.410	1.00	32.82	B	N
ATOM	6608	CA	PHE	113	115.678	81.965	40.401	1.00	31.84	B	C
ATOM	6609	CB	PHE	113	115.185	82.165	38.969	1.00	31.95	B	C
ATOM	6610	CG	PHE	113	115.948	83.204	38.208	1.00	34.16	B	C
ATOM	6611	CD1	PHE	113	117.150	82.886	37.587	1.00	35.65	B	C
ATOM	6612	CD2	PHE	113	115.475	84.508	38.124	1.00	35.41	B	C
ATOM	6613	CE1	PHE	113	117.872	83.853	36.893	1.00	36.00	B	C
ATOM	6614	CE2	PHE	113	116.185	85.479	37.436	1.00	35.02	B	C

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## FIG. 4 - 136

(Continued)

ATOM	6615	CZ	PHE	113	117.386	85.152	36.819	1.00	35.71	B	C
ATOM	6616	C	PHE	113	114.831	80.896	41.058	1.00	30.65	B	C
ATOM	6617	O	PHE	113	115.308	79.829	41.425	1.00	30.90	B	O
ATOM	6618	N	ILE	114	113.557	81.205	41.219	1.00	30.09	B	N
ATOM	6619	CA	ILE	114	112.630	80.258	41.791	1.00	29.81	B	C
ATOM	6620	CB	ILE	114	112.394	80.504	43.293	1.00	28.60	B	C
ATOM	6621	CG2	ILE	114	111.911	81.915	43.529	1.00	29.81	B	C
ATOM	6622	CG1	ILE	114	111.378	79.490	43.813	1.00	30.57	B	C
ATOM	6623	CD1	ILE	114	111.336	79.367	45.325	1.00	33.23	B	C
ATOM	6624	C	ILE	114	111.336	80.403	41.019	1.00	29.79	B	C
ATOM	6625	O	ILE	114	110.895	81.508	40.715	1.00	28.83	B	O
ATOM	6626	N	LEU	115	110.756	79.265	40.671	1.00	30.43	B	N
ATOM	6627	CA	LEU	115	109.516	79.223	39.925	1.00	29.05	B	C
ATOM	6628	CB	LEU	115	109.596	78.108	38.890	1.00	28.31	B	C
ATOM	6629	CG	LEU	115	108.449	77.898	37.912	1.00	28.22	B	C
ATOM	6630	CD1	LEU	115	108.425	79.001	36.872	1.00	28.47	B	C
ATOM	6631	CD2	LEU	115	108.645	76.553	37.245	1.00	29.52	B	C
ATOM	6632	C	LEU	115	108.424	78.923	40.932	1.00	29.59	B	C
ATOM	6633	O	LEU	115	108.370	77.824	41.483	1.00	30.72	B	O
ATOM	6634	N	LEU	116	107.568	79.901	41.196	1.00	30.29	B	N
ATOM	6635	CA	LEU	116	106.479	79.699	42.142	1.00	30.17	B	C
ATOM	6636	CB	LEU	116	106.129	81.001	42.861	1.00	31.28	B	C
ATOM	6637	CG	LEU	116	107.277	81.741	43.544	1.00	33.66	B	C
ATOM	6638	CD1	LEU	116	106.732	82.988	44.229	1.00	33.41	B	C
ATOM	6639	CD2	LEU	116	107.957	80.821	44.552	1.00	34.07	B	C
ATOM	6640	C	LEU	116	105.270	79.215	41.369	1.00	30.44	B	C
ATOM	6641	O	LEU	116	104.835	79.845	40.401	1.00	30.69	B	O
ATOM	6642	N	GLU	117	104.724	78.091	41.804	1.00	30.37	B	N
ATOM	6643	CA	GLU	117	103.563	77.513	41.159	1.00	29.50	B	C
ATOM	6644	CB	GLU	117	103.813	76.017	40.963	1.00	30.63	B	C
ATOM	6645	CG	GLU	117	102.671	75.210	40.368	1.00	32.07	B	C
ATOM	6646	CD	GLU	117	103.023	73.728	40.270	1.00	33.58	B	C
ATOM	6647	OE1	GLU	117	103.772	73.341	39.340	1.00	32.53	B	O
ATOM	6648	OE2	GLU	117	102.566	72.956	41.140	1.00	32.35	B	O
ATOM	6649	C	GLU	117	102.312	77.756	42.009	1.00	29.67	B	C
ATOM	6650	O	GLU	117	102.333	77.583	43.228	1.00	27.89	B	O
ATOM	6651	N	TYR	118	101.235	78.184	41.355	1.00	29.27	B	N
ATOM	6652	CA	TYR	118	99.966	78.423	42.026	1.00	28.00	B	C
ATOM	6653	CB	TYR	118	99.928	79.818	42.643	1.00	29.37	B	C
ATOM	6654	CG	TYR	118	100.036	80.955	41.659	1.00	29.69	B	C
ATOM	6655	CD1	TYR	118	101.256	81.301	41.092	1.00	30.04	B	C
ATOM	6656	CE1	TYR	118	101.355	82.373	40.210	1.00	31.36	B	C
ATOM	6657	CD2	TYR	118	98.915	81.703	41.316	1.00	30.41	B	C
ATOM	6658	CE2	TYR	118	99.003	82.768	40.439	1.00	31.17	B	C
ATOM	6659	CZ	TYR	118	100.222	83.101	39.891	1.00	31.56	B	C
ATOM	6660	OH	TYR	118	100.298	84.179	39.039	1.00	33.43	B	O
ATOM	6661	C	TYR	118	98.814	78.240	41.038	1.00	27.66	B	C
ATOM	6662	O	TYR	118	99.046	77.917	39.874	1.00	26.73	B	O
ATOM	6663	N	ASN	119	97.582	78.450	41.499	1.00	27.22	B	N

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## FIG. 4 - 137

(Continued)

ATOM	6664	CA	ASN	119	96.397	78.261	40.659	1.00	27.10	B	C
ATOM	6665	CB	ASN	119	96.422	79.203	39.449	1.00	27.22	B	C
ATOM	6666	CG	ASN	119	95.918	80.599	39.777	1.00	27.62	B	C
ATOM	6667	OD1	ASN	119	94.905	80.761	40.456	1.00	26.76	B	O
ATOM	6668	ND2	ASN	119	96.613	81.612	39.277	1.00	25.87	B	N
ATOM	6669	C	ASN	119	96.342	76.810	40.171	1.00	27.88	B	C
ATOM	6670	O	ASN	119	95.923	76.534	39.045	1.00	27.93	B	O
ATOM	6671	N	TYR	120	96.771	75.888	41.028	1.00	27.57	B	N
ATOM	6672	CA	TYR	120	96.795	74.466	40.702	1.00	29.01	B	C
ATOM	6673	CB	TYR	120	97.396	73.669	41.866	1.00	30.85	B	C
ATOM	6674	CG	TYR	120	97.421	72.171	41.635	1.00	32.83	B	C
ATOM	6675	CD1	TYR	120	98.466	71.568	40.940	1.00	33.76	B	C
ATOM	6676	CE1	TYR	120	98.484	70.190	40.717	1.00	35.03	B	C
ATOM	6677	CD2	TYR	120	96.389	71.358	42.100	1.00	34.41	B	C
ATOM	6678	CE2	TYR	120	96.394	69.981	41.880	1.00	34.35	B	C
ATOM	6679	CZ	TYR	120	97.444	69.403	41.191	1.00	35.47	B	C
ATOM	6680	OH	TYR	120	97.462	68.039	40.987	1.00	35.56	B	O
ATOM	6681	C	TYR	120	95.431	73.863	40.364	1.00	29.17	B	C
ATOM	6682	O	TYR	120	94.458	74.034	41.099	1.00	31.09	B	O
ATOM	6683	N	VAL	121	95.368	73.148	39.248	1.00	27.53	B	N
ATOM	6684	CA	VAL	121	94.136	72.487	38.842	1.00	25.45	B	C
ATOM	6685	CB	VAL	121	93.358	73.296	37.785	1.00	25.23	B	C
ATOM	6686	CG1	VAL	121	92.105	72.534	37.376	1.00	22.18	B	C
ATOM	6687	CG2	VAL	121	92.974	74.666	38.354	1.00	21.81	B	C
ATOM	6688	C	VAL	121	94.527	71.130	38.275	1.00	24.99	B	C
ATOM	6689	O	VAL	121	95.188	71.031	37.242	1.00	24.18	B	O
ATOM	6690	N	LYS	122	94.124	70.082	38.977	1.00	24.16	B	N
ATOM	6691	CA	LYS	122	94.464	68.735	38.570	1.00	24.24	B	C
ATOM	6692	CB	LYS	122	94.295	67.780	39.754	1.00	23.05	B	C
ATOM	6693	CG	LYS	122	94.510	66.327	39.390	1.00	20.04	B	C
ATOM	6694	CD	LYS	122	94.356	65.416	40.589	1.00	20.19	B	C
ATOM	6695	CE	LYS	122	94.402	63.950	40.161	1.00	20.85	B	C
ATOM	6696	NZ	LYS	122	93.363	63.632	39.136	1.00	18.96	B	N
ATOM	6697	C	LYS	122	93.692	68.180	37.387	1.00	24.10	B	C
ATOM	6698	O	LYS	122	92.516	68.488	37.189	1.00	23.23	B	O
ATOM	6699	N	GLN	123	94.384	67.368	36.592	1.00	23.36	B	N
ATOM	6700	CA	GLN	123	93.758	66.691	35.472	1.00	21.22	B	C
ATOM	6701	CB	GLN	123	94.455	67.007	34.145	1.00	20.62	B	C
ATOM	6702	CG	GLN	123	93.689	66.433	32.948	1.00	23.42	B	C
ATOM	6703	CD	GLN	123	94.242	66.857	31.591	1.00	24.37	B	C
ATOM	6704	OE1	GLN	123	95.399	66.606	31.275	1.00	26.71	B	O
ATOM	6705	NE2	GLN	123	93.402	67.493	30.779	1.00	23.80	B	N
ATOM	6706	C	GLN	123	93.856	65.194	35.805	1.00	20.06	B	C
ATOM	6707	O	GLN	123	93.258	64.741	36.786	1.00	17.04	B	O
ATOM	6708	N	TRP	124	94.630	64.438	35.030	1.00	17.49	B	N
ATOM	6709	CA	TRP	124	94.753	63.009	35.276	1.00	16.75	B	C
ATOM	6710	CB	TRP	124	95.165	62.298	33.984	1.00	16.19	B	C
ATOM	6711	CG	TRP	124	94.351	62.735	32.797	1.00	18.11	B	C
ATOM	6712	CD2	TRP	124	92.939	63.014	32.764	1.00	17.55	B	C

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(Continued)

## FIG. 4 - 138

ATOM	6713	CE2	TRP	124	92.630	63.449	31.455	1.00	16.84	B	C
ATOM	6714	CE3	TRP	124	91.909	62.942	33.713	1.00	17.02	B	C
ATOM	6715	CD1	TRP	124	94.819	62.999	31.539	1.00	19.00	B	C
ATOM	6716	NE1	TRP	124	93.794	63.429	30.731	1.00	18.26	B	N
ATOM	6717	CZ2	TRP	124	91.331	63.815	31.067	1.00	15.16	B	C
ATOM	6718	CZ3	TRP	124	90.615	63.305	33.326	1.00	16.85	B	C
ATOM	6719	CH2	TRP	124	90.342	63.737	32.011	1.00	16.12	B	C
ATOM	6720	C	TRP	124	95.718	62.679	36.427	1.00	17.28	B	C
ATOM	6721	O	TRP	124	95.816	63.437	37.397	1.00	17.74	B	O
ATOM	6722	N	ARG	125	96.430	61.560	36.339	1.00	15.31	B	N
ATOM	6723	CA	ARG	125	97.317	61.185	37.429	1.00	16.66	B	C
ATOM	6724	CB	ARG	125	97.666	59.702	37.323	1.00	16.96	B	C
ATOM	6725	CG	ARG	125	98.908	59.288	38.076	1.00	18.35	B	C
ATOM	6726	CD	ARG	125	98.689	57.987	38.794	1.00	18.85	B	C
ATOM	6727	NE	ARG	125	98.049	56.965	37.972	1.00	18.57	B	N
ATOM	6728	CZ	ARG	125	97.547	55.842	38.475	1.00	17.58	B	C
ATOM	6729	NH1	ARG	125	96.972	54.944	37.693	1.00	16.96	B	N
ATOM	6730	NH2	ARG	125	97.626	55.621	39.776	1.00	17.03	B	N
ATOM	6731	C	ARG	125	98.582	62.027	37.568	1.00	18.54	B	C
ATOM	6732	O	ARG	125	99.075	62.227	38.674	1.00	18.06	B	O
ATOM	6733	N	HIS	126	99.099	62.533	36.454	1.00	20.06	B	N
ATOM	6734	CA	HIS	126	100.300	63.353	36.487	1.00	18.20	B	C
ATOM	6735	CB	HIS	126	101.391	62.673	35.673	1.00	18.72	B	C
ATOM	6736	CG	HIS	126	101.721	61.295	36.151	1.00	19.88	B	C
ATOM	6737	CD2	HIS	126	101.519	60.084	35.581	1.00	20.06	B	C
ATOM	6738	ND1	HIS	126	102.341	61.054	37.360	1.00	17.75	B	N
ATOM	6739	CE1	HIS	126	102.510	59.753	37.512	1.00	19.55	B	C
ATOM	6740	NE2	HIS	126	102.019	59.142	36.447	1.00	22.65	B	N
ATOM	6741	C	HIS	126	100.079	64.772	35.966	1.00	18.28	B	C
ATOM	6742	O	HIS	126	100.692	65.716	36.462	1.00	18.27	B	O
ATOM	6743	N	SER	127	99.204	64.921	34.974	1.00	16.08	B	N
ATOM	6744	CA	SER	127	98.936	66.230	34.382	1.00	16.78	B	C
ATOM	6745	CB	SER	127	98.209	66.070	33.037	1.00	15.96	B	C
ATOM	6746	OG	SER	127	96.999	65.349	33.179	1.00	17.80	B	O
ATOM	6747	C	SER	127	98.151	67.203	35.261	1.00	16.75	B	C
ATOM	6748	O	SER	127	97.523	66.816	36.247	1.00	17.88	B	O
ATOM	6749	N	TYR	128	98.205	68.473	34.873	1.00	15.65	B	N
ATOM	6750	CA	TYR	128	97.520	69.556	35.559	1.00	17.91	B	C
ATOM	6751	CB	TYR	128	97.815	69.506	37.060	1.00	17.70	B	C
ATOM	6752	CG	TYR	128	99.253	69.796	37.444	1.00	17.20	B	C
ATOM	6753	CD1	TYR	128	99.725	71.107	37.540	1.00	16.17	B	C
ATOM	6754	CE1	TYR	128	101.036	71.375	37.927	1.00	16.04	B	C
ATOM	6755	CD2	TYR	128	100.135	68.759	37.739	1.00	17.12	B	C
ATOM	6756	CE2	TYR	128	101.449	69.016	38.123	1.00	15.90	B	C
ATOM	6757	CZ	TYR	128	101.891	70.322	38.216	1.00	17.19	B	C
ATOM	6758	OH	TYR	128	103.190	70.572	38.603	1.00	20.16	B	O
ATOM	6759	C	TYR	128	97.977	70.897	34.992	1.00	19.77	B	C
ATOM	6760	O	TYR	128	98.970	70.972	34.268	1.00	21.70	B	O
ATOM	6761	N	THR	129	97.239	71.955	35.291	1.00	20.48	B	N

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## FIG. 4 - 139

(Continued)

ATOM	6762	CA	THR	129	97.647	73.276	34.840	1.00	22.26	B	C
ATOM	6763	CB	THR	129	96.599	73.968	33.950	1.00	23.04	B	C
ATOM	6764	OG1	THR	129	95.353	74.045	34.652	1.00	24.93	B	O
ATOM	6765	CG2	THR	129	96.428	73.213	32.634	1.00	22.70	B	C
ATOM	6766	C	THR	129	97.856	74.136	36.069	1.00	22.23	B	C
ATOM	6767	O	THR	129	97.462	73.765	37.182	1.00	20.98	B	O
ATOM	6768	N	ALA	130	98.474	75.289	35.854	1.00	22.77	B	N
ATOM	6769	CA	ALA	130	98.754	76.222	36.926	1.00	23.41	B	C
ATOM	6770	CB	ALA	130	99.789	75.631	37.859	1.00	19.73	B	C
ATOM	6771	C	ALA	130	99.269	77.525	36.338	1.00	26.66	B	C
ATOM	6772	O	ALA	130	99.514	77.632	35.133	1.00	27.20	B	O
ATOM	6773	N	SER	131	99.414	78.523	37.199	1.00	29.67	B	N
ATOM	6774	CA	SER	131	99.934	79.818	36.796	1.00	30.14	B	C
ATOM	6775	CB	SER	131	99.056	80.948	37.333	1.00	30.56	B	C
ATOM	6776	OG	SER	131	97.713	80.775	36.913	1.00	32.67	B	O
ATOM	6777	C	SER	131	101.290	79.851	37.463	1.00	31.00	B	C
ATOM	6778	O	SER	131	101.448	79.334	38.569	1.00	30.79	B	O
ATOM	6779	N	TYR	132	102.272	80.438	36.792	1.00	32.02	B	N
ATOM	6780	CA	TYR	132	103.611	80.506	37.347	1.00	31.40	B	C
ATOM	6781	CB	TYR	132	104.558	79.634	36.519	1.00	28.72	B	C
ATOM	6782	CG	TYR	132	104.179	78.174	36.516	1.00	26.74	B	C
ATOM	6783	CD1	TYR	132	103.082	77.721	35.791	1.00	26.31	B	C
ATOM	6784	CE1	TYR	132	102.696	76.383	35.834	1.00	26.45	B	C
ATOM	6785	CD2	TYR	132	104.887	77.250	37.283	1.00	26.58	B	C
ATOM	6786	CE2	TYR	132	104.510	75.911	37.332	1.00	24.63	B	C
ATOM	6787	CZ	TYR	132	103.415	75.486	36.609	1.00	25.59	B	C
ATOM	6788	OH	TYR	132	103.023	74.171	36.677	1.00	25.63	B	O
ATOM	6789	C	TYR	132	104.143	81.929	37.411	1.00	32.91	B	C
ATOM	6790	O	TYR	132	103.743	82.790	36.636	1.00	34.01	B	O
ATOM	6791	N	ASP	133	105.041	82.165	38.358	1.00	35.11	B	N
ATOM	6792	CA	ASP	133	105.674	83.465	38.539	1.00	36.35	B	C
ATOM	6793	CB	ASP	133	104.954	84.287	39.614	1.00	38.51	B	C
ATOM	6794	CG	ASP	133	103.732	85.008	39.074	1.00	41.22	B	C
ATOM	6795	OD1	ASP	133	102.805	84.332	38.580	1.00	42.20	B	O
ATOM	6796	OD2	ASP	133	103.702	86.253	39.139	1.00	42.84	B	O
ATOM	6797	C	ASP	133	107.112	83.228	38.954	1.00	35.61	B	C
ATOM	6798	O	ASP	133	107.385	82.438	39.855	1.00	35.76	B	O
ATOM	6799	N	ILE	134	108.031	83.908	38.285	1.00	35.21	B	N
ATOM	6800	CA	ILE	134	109.444	83.764	38.585	1.00	34.01	B	C
ATOM	6801	CB	ILE	134	110.267	83.750	37.287	1.00	33.62	B	C
ATOM	6802	CG2	ILE	134	111.718	83.392	37.593	1.00	31.90	B	C
ATOM	6803	CG1	ILE	134	109.649	82.737	36.312	1.00	32.72	B	C
ATOM	6804	CD1	ILE	134	110.204	82.794	34.909	1.00	31.29	B	C
ATOM	6805	C	ILE	134	109.887	84.911	39.483	1.00	34.02	B	C
ATOM	6806	O	ILE	134	109.521	86.065	39.261	1.00	33.25	B	O
ATOM	6807	N	TYR	135	110.662	84.573	40.507	1.00	35.09	B	N
ATOM	6808	CA	TYR	135	111.167	85.539	41.475	1.00	36.09	B	C
ATOM	6809	CB	TYR	135	110.657	85.174	42.868	1.00	36.02	B	C
ATOM	6810	CG	TYR	135	111.222	86.011	44.000	1.00	36.66	B	C

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## FIG. 4 - 140

(Continued)

ATOM	6811	CD1	TYR	135	110.635	87.222	44.363	1.00	34.73	B	C
ATOM	6812	CE1	TYR	135	111.134	87.971	45.424	1.00	34.55	B	C
ATOM	6813	CD2	TYR	135	112.332	85.573	44.729	1.00	35.12	B	C
ATOM	6814	CE2	TYR	135	112.839	86.316	45.786	1.00	35.07	B	C
ATOM	6815	CZ	TYR	135	112.235	87.515	46.131	1.00	35.31	B	C
ATOM	6816	OH	TYR	135	112.740	88.258	47.179	1.00	35.05	B	O
ATOM	6817	C	TYR	135	112.688	85.511	41.470	1.00	38.19	B	C
ATOM	6818	O	TYR	135	113.293	84.517	41.873	1.00	37.81	B	O
ATOM	6819	N	ASP	136	113.304	86.600	41.014	1.00	40.56	B	N
ATOM	6820	CA	ASP	136	114.759	86.692	40.965	1.00	42.09	B	C
ATOM	6821	CB	ASP	136	115.187	87.969	40.237	1.00	42.45	B	C
ATOM	6822	CG	ASP	136	116.690	88.051	40.030	1.00	43.61	B	C
ATOM	6823	OD1	ASP	136	117.107	88.577	38.978	1.00	45.53	B	O
ATOM	6824	OD2	ASP	136	117.456	87.602	40.911	1.00	41.77	B	O
ATOM	6825	C	ASP	136	115.316	86.679	42.382	1.00	43.14	B	C
ATOM	6826	O	ASP	136	114.972	87.522	43.209	1.00	42.49	B	O
ATOM	6827	N	LEU	137	116.181	85.713	42.656	1.00	44.92	B	N
ATOM	6828	CA	LEU	137	116.761	85.577	43.978	1.00	48.26	B	C
ATOM	6829	CB	LEU	137	117.219	84.135	44.182	1.00	48.88	B	C
ATOM	6830	CG	LEU	137	116.058	83.136	44.117	1.00	49.07	B	C
ATOM	6831	CD1	LEU	137	116.582	81.716	43.991	1.00	50.17	B	C
ATOM	6832	CD2	LEU	137	115.199	83.291	45.361	1.00	48.91	B	C
ATOM	6833	C	LEU	137	117.908	86.544	44.228	1.00	50.19	B	C
ATOM	6834	O	LEU	137	118.309	86.750	45.370	1.00	51.45	B	O
ATOM	6835	N	ASN	138	118.429	87.139	43.160	1.00	52.26	B	N
ATOM	6836	CA	ASN	138	119.522	88.096	43.280	1.00	53.21	B	C
ATOM	6837	CB	ASN	138	120.330	88.151	41.983	1.00	54.36	B	C
ATOM	6838	CG	ASN	138	120.728	86.775	41.484	1.00	56.39	B	C
ATOM	6839	OD1	ASN	138	121.232	85.945	42.244	1.00	57.23	B	O
ATOM	6840	ND2	ASN	138	120.512	86.530	40.194	1.00	56.67	B	N
ATOM	6841	C	ASN	138	118.935	89.472	43.567	1.00	54.11	B	C
ATOM	6842	O	ASN	138	119.259	90.101	44.571	1.00	54.39	B	O
ATOM	6843	N	LYS	139	118.064	89.929	42.675	1.00	55.06	B	N
ATOM	6844	CA	LYS	139	117.417	91.228	42.814	1.00	56.16	B	C
ATOM	6845	CB	LYS	139	116.807	91.657	41.480	1.00	56.75	B	C
ATOM	6846	CG	LYS	139	117.726	91.520	40.290	1.00	58.34	B	C
ATOM	6847	CD	LYS	139	116.996	91.874	39.006	1.00	59.63	B	C
ATOM	6848	CE	LYS	139	117.887	91.650	37.793	1.00	61.32	B	C
ATOM	6849	NZ	LYS	139	117.196	91.995	36.518	1.00	62.59	B	N
ATOM	6850	C	LYS	139	116.302	91.183	43.857	1.00	56.78	B	C
ATOM	6851	O	LYS	139	115.669	92.202	44.139	1.00	57.22	B	O
ATOM	6852	N	ARG	140	116.061	90.006	44.425	1.00	57.14	B	N
ATOM	6853	CA	ARG	140	114.994	89.838	45.409	1.00	57.44	B	C
ATOM	6854	CB	ARG	140	115.433	90.341	46.787	1.00	58.40	B	C
ATOM	6855	CG	ARG	140	116.063	89.260	47.649	1.00	61.65	B	C
ATOM	6856	CD	ARG	140	116.091	89.658	49.116	1.00	64.17	B	C
ATOM	6857	NE	ARG	140	116.578	88.575	49.972	1.00	67.20	B	N
ATOM	6858	CZ	ARG	140	115.979	87.394	50.112	1.00	68.02	B	C
ATOM	6859	NH1	ARG	140	114.857	87.124	49.453	1.00	68.21	B	N

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## FIG. 4 - 141

(Continued)

ATOM	6860	NH2	ARG	140	116.507	86.478	50.911	1.00	68.11	B	N
ATOM	6861	C	ARG	140	113.697	90.537	44.994	1.00	56.16	B	C
ATOM	6862	O	ARG	140	113.067	91.225	45.795	1.00	56.03	B	O
ATOM	6863	N	GLN	141	113.315	90.363	43.733	1.00	54.56	B	N
ATOM	6864	CA	GLN	141	112.088	90.947	43.205	1.00	53.90	B	C
ATOM	6865	CB	GLN	141	112.367	92.292	42.522	1.00	55.16	B	C
ATOM	6866	CG	GLN	141	113.166	92.203	41.227	1.00	57.86	B	C
ATOM	6867	CD	GLN	141	113.078	93.477	40.400	1.00	59.30	B	C
ATOM	6868	OE1	GLN	141	113.414	94.562	40.875	1.00	60.96	B	O
ATOM	6869	NE2	GLN	141	112.620	93.350	39.158	1.00	58.33	B	N
ATOM	6870	C	GLN	141	111.500	89.965	42.198	1.00	52.05	B	C
ATOM	6871	O	GLN	141	112.230	89.362	41.418	1.00	52.50	B	O
ATOM	6872	N	LEU	142	110.186	89.794	42.213	1.00	50.43	B	N
ATOM	6873	CA	LEU	142	109.564	88.861	41.284	1.00	48.86	B	C
ATOM	6874	CB	LEU	142	108.196	88.415	41.815	1.00	48.84	B	C
ATOM	6875	CG	LEU	142	107.024	89.395	41.857	1.00	48.67	B	C
ATOM	6876	CD1	LEU	142	106.354	89.442	40.489	1.00	49.83	B	C
ATOM	6877	CD2	LEU	142	106.014	88.940	42.905	1.00	47.77	B	C
ATOM	6878	C	LEU	142	109.423	89.467	39.896	1.00	47.71	B	C
ATOM	6879	O	LEU	142	108.890	90.564	39.736	1.00	48.46	B	O
ATOM	6880	N	ILE	143	109.917	88.752	38.891	1.00	45.67	B	N
ATOM	6881	CA	ILE	143	109.835	89.226	37.520	1.00	42.98	B	C
ATOM	6882	CB	ILE	143	110.442	88.208	36.535	1.00	42.34	B	C
ATOM	6883	CG2	ILE	143	110.204	88.659	35.099	1.00	41.35	B	C
ATOM	6884	CG1	ILE	143	111.937	88.055	36.810	1.00	41.52	B	C
ATOM	6885	CD1	ILE	143	112.675	87.257	35.755	1.00	42.12	B	C
ATOM	6886	C	ILE	143	108.385	89.481	37.131	1.00	42.92	B	C
ATOM	6887	O	ILE	143	107.522	88.617	37.292	1.00	41.84	B	O
ATOM	6888	N	THR	144	108.128	90.680	36.620	1.00	43.57	B	N
ATOM	6889	CA	THR	144	106.789	91.065	36.202	1.00	44.05	B	C
ATOM	6890	CB	THR	144	106.332	92.344	36.915	1.00	42.77	B	C
ATOM	6891	OG1	THR	144	107.329	93.358	36.760	1.00	45.33	B	O
ATOM	6892	CG2	THR	144	106.124	92.080	38.388	1.00	43.31	B	C
ATOM	6893	C	THR	144	106.716	91.294	34.701	1.00	44.53	B	C
ATOM	6894	O	THR	144	105.689	91.729	34.186	1.00	46.08	B	O
ATOM	6895	N	GLU	145	107.802	90.988	34.001	1.00	45.05	B	N
ATOM	6896	CA	GLU	145	107.857	91.168	32.557	1.00	46.88	B	C
ATOM	6897	CB	GLU	145	109.069	92.031	32.202	1.00	50.14	B	C
ATOM	6898	CG	GLU	145	109.148	93.319	33.007	1.00	55.05	B	C
ATOM	6899	CD	GLU	145	110.429	94.094	32.760	1.00	57.57	B	C
ATOM	6900	OE1	GLU	145	110.696	94.443	31.591	1.00	60.26	B	O
ATOM	6901	OE2	GLU	145	111.167	94.357	33.737	1.00	59.47	B	O
ATOM	6902	C	GLU	145	107.946	89.822	31.834	1.00	46.87	B	C
ATOM	6903	O	GLU	145	108.648	88.916	32.286	1.00	46.76	B	O
ATOM	6904	N	GLU	146	107.236	89.695	30.714	1.00	46.37	B	N
ATOM	6905	CA	GLU	146	107.241	88.458	29.932	1.00	45.82	B	C
ATOM	6906	CB	GLU	146	108.592	88.284	29.232	1.00	46.20	B	C
ATOM	6907	CG	GLU	146	108.916	89.321	28.163	1.00	45.55	B	C
ATOM	6908	CD	GLU	146	108.011	89.217	26.948	1.00	45.65	B	C

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## FIG. 4 - 142

(Continued)

ATOM	6909	OE1	GLU	146	107.685	88.081	26.543	1.00	45.03	B	O
ATOM	6910	OE2	GLU	146	107.641	90.269	26.387	1.00	45.44	B	O
ATOM	6911	C	GLU	146	106.978	87.241	30.821	1.00	46.25	B	C
ATOM	6912	O	GLU	146	107.805	86.334	30.912	1.00	47.62	B	O
ATOM	6913	N	ARG	147	105.823	87.221	31.474	1.00	44.79	B	N
ATOM	6914	CA	ARG	147	105.475	86.119	32.360	1.00	43.34	B	C
ATOM	6915	CB	ARG	147	104.469	86.595	33.410	1.00	44.21	B	C
ATOM	6916	CG	ARG	147	104.998	87.678	34.320	1.00	46.85	B	C
ATOM	6917	CD	ARG	147	103.995	88.007	35.410	1.00	49.84	B	C
ATOM	6918	NE	ARG	147	102.805	88.651	34.866	1.00	53.22	B	N
ATOM	6919	CZ	ARG	147	101.733	88.970	35.584	1.00	54.21	B	C
ATOM	6920	NH1	ARG	147	101.696	88.699	36.884	1.00	53.97	B	N
ATOM	6921	NH2	ARG	147	100.701	89.569	34.999	1.00	54.56	B	N
ATOM	6922	C	ARG	147	104.905	84.894	31.648	1.00	41.06	B	C
ATOM	6923	O	ARG	147	104.304	84.996	30.580	1.00	41.00	B	O
ATOM	6924	N	ILE	148	105.103	83.732	32.259	1.00	38.31	B	N
ATOM	6925	CA	ILE	148	104.590	82.485	31.721	1.00	35.74	B	C
ATOM	6926	CB	ILE	148	105.019	81.305	32.616	1.00	35.07	B	C
ATOM	6927	CG2	ILE	148	104.458	79.996	32.073	1.00	34.22	B	C
ATOM	6928	CG1	ILE	148	106.549	81.255	32.679	1.00	33.62	B	C
ATOM	6929	CD1	ILE	148	107.104	80.131	33.517	1.00	34.57	B	C
ATOM	6930	C	ILE	148	103.069	82.641	31.709	1.00	34.54	B	C
ATOM	6931	O	ILE	148	102.492	83.155	32.664	1.00	35.51	B	O
ATOM	6932	N	PRO	149	102.401	82.199	30.631	1.00	32.42	B	N
ATOM	6933	CD	PRO	149	102.929	81.387	29.525	1.00	30.91	B	C
ATOM	6934	CA	PRO	149	100.942	82.321	30.526	1.00	31.27	B	C
ATOM	6935	CB	PRO	149	100.632	81.762	29.134	1.00	31.04	B	C
ATOM	6936	CG	PRO	149	101.963	81.707	28.437	1.00	31.84	B	C
ATOM	6937	C	PRO	149	100.187	81.549	31.592	1.00	31.48	B	C
ATOM	6938	O	PRO	149	100.733	80.643	32.221	1.00	30.85	B	O
ATOM	6939	N	ASN	150	98.927	81.919	31.794	1.00	31.40	B	N
ATOM	6940	CA	ASN	150	98.085	81.206	32.744	1.00	31.30	B	C
ATOM	6941	CB	ASN	150	96.832	82.019	33.108	1.00	31.58	B	C
ATOM	6942	CG	ASN	150	97.086	83.037	34.211	1.00	32.97	B	C
ATOM	6943	OD1	ASN	150	97.676	82.715	35.244	1.00	31.95	B	O
ATOM	6944	ND2	ASN	150	96.624	84.271	34.004	1.00	33.51	B	N
ATOM	6945	C	ASN	150	97.673	79.929	32.013	1.00	30.52	B	C
ATOM	6946	O	ASN	150	97.722	79.864	30.777	1.00	29.37	B	O
ATOM	6947	N	ASN	151	97.269	78.917	32.768	1.00	30.16	B	N
ATOM	6948	CA	ASN	151	96.859	77.657	32.170	1.00	29.53	B	C
ATOM	6949	CB	ASN	151	95.715	77.881	31.186	1.00	33.04	B	C
ATOM	6950	CG	ASN	151	94.489	78.474	31.850	1.00	36.73	B	C
ATOM	6951	OD1	ASN	151	94.530	79.586	32.376	1.00	38.47	B	O
ATOM	6952	ND2	ASN	151	93.389	77.729	31.831	1.00	40.28	B	N
ATOM	6953	C	ASN	151	98.023	76.997	31.452	1.00	28.44	B	C
ATOM	6954	O	ASN	151	97.856	76.412	30.382	1.00	27.56	B	O
ATOM	6955	N	THR	152	99.212	77.111	32.035	1.00	26.08	B	N
ATOM	6956	CA	THR	152	100.384	76.489	31.452	1.00	24.37	B	C
ATOM	6957	CB	THR	152	101.682	77.069	32.046	1.00	25.30	B	C

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## FIG. 4 - 143

(Continued)

ATOM	6958	OG1	THR	152	101.862	78.407	31.566	1.00	25.07	B	O
ATOM	6959	CG2	THR	152	102.882	76.231	31.643	1.00	24.98	B	C
ATOM	6960	C	THR	152	100.257	75.012	31.791	1.00	22.65	B	C
ATOM	6961	O	THR	152	99.908	74.652	32.912	1.00	21.72	B	O
ATOM	6962	N	GLN	153	100.531	74.160	30.815	1.00	21.08	B	N
ATOM	6963	CA	GLN	153	100.407	72.730	31.010	1.00	20.14	B	C
ATOM	6964	CB	GLN	153	100.023	72.081	29.691	1.00	20.22	B	C
ATOM	6965	CG	GLN	153	98.688	72.573	29.166	1.00	20.23	B	C
ATOM	6966	CD	GLN	153	98.577	72.461	27.669	1.00	21.29	B	C
ATOM	6967	OE1	GLN	153	99.365	73.054	26.939	1.00	24.47	B	O
ATOM	6968	NE2	GLN	153	97.600	71.703	27.200	1.00	20.51	B	N
ATOM	6969	C	GLN	153	101.650	72.076	31.578	1.00	20.86	B	C
ATOM	6970	O	GLN	153	101.574	70.996	32.154	1.00	22.44	B	O
ATOM	6971	N	TRP	154	102.794	72.729	31.422	1.00	20.43	B	N
ATOM	6972	CA	TRP	154	104.043	72.189	31.934	1.00	18.53	B	C
ATOM	6973	CB	TRP	154	104.387	70.868	31.234	1.00	18.88	B	C
ATOM	6974	CG	TRP	154	105.678	70.257	31.719	1.00	19.59	B	C
ATOM	6975	CD2	TRP	154	105.891	69.559	32.955	1.00	17.98	B	C
ATOM	6976	CE2	TRP	154	107.261	69.232	33.019	1.00	19.74	B	C
ATOM	6977	CE3	TRP	154	105.058	69.184	34.015	1.00	16.08	B	C
ATOM	6978	CD1	TRP	154	106.893	70.316	31.101	1.00	20.53	B	C
ATOM	6979	NE1	TRP	154	107.849	69.705	31.877	1.00	22.41	B	N
ATOM	6980	CZ2	TRP	154	107.819	68.545	34.104	1.00	18.81	B	C
ATOM	6981	CZ3	TRP	154	105.614	68.502	35.097	1.00	14.46	B	C
ATOM	6982	CH2	TRP	154	106.981	68.191	35.130	1.00	14.70	B	C
ATOM	6983	C	TRP	154	105.172	73.186	31.757	1.00	18.38	B	C
ATOM	6984	O	TRP	154	105.159	74.005	30.840	1.00	17.07	B	O
ATOM	6985	N	VAL	155	106.139	73.118	32.658	1.00	18.34	B	N
ATOM	6986	CA	VAL	155	107.280	74.010	32.627	1.00	20.45	B	C
ATOM	6987	CB	VAL	155	107.030	75.298	33.457	1.00	21.97	B	C
ATOM	6988	CG1	VAL	155	106.881	74.954	34.937	1.00	21.60	B	C
ATOM	6989	CG2	VAL	155	108.180	76.281	33.260	1.00	20.89	B	C
ATOM	6990	C	VAL	155	108.439	73.255	33.236	1.00	21.60	B	C
ATOM	6991	O	VAL	155	108.241	72.379	34.075	1.00	21.26	B	O
ATOM	6992	N	THR	156	109.647	73.590	32.806	1.00	22.32	B	N
ATOM	6993	CA	THR	156	110.826	72.929	33.325	1.00	23.44	B	C
ATOM	6994	CB	THR	156	111.028	71.569	32.677	1.00	24.53	B	C
ATOM	6995	OG1	THR	156	112.350	71.113	32.972	1.00	25.64	B	O
ATOM	6996	CG2	THR	156	110.856	71.662	31.166	1.00	25.95	B	C
ATOM	6997	C	THR	156	112.092	73.727	33.094	1.00	24.37	B	C
ATOM	6998	O	THR	156	112.305	74.274	32.010	1.00	25.56	B	O
ATOM	6999	N	TRP	157	112.929	73.795	34.123	1.00	23.78	B	N
ATOM	7000	CA	TRP	157	114.192	74.500	34.021	1.00	22.95	B	C
ATOM	7001	CB	TRP	157	114.848	74.650	35.399	1.00	22.02	B	C
ATOM	7002	CG	TRP	157	114.239	75.678	36.293	1.00	21.39	B	C
ATOM	7003	CD2	TRP	157	114.197	77.091	36.070	1.00	22.25	B	C
ATOM	7004	CE2	TRP	157	113.533	77.668	37.177	1.00	23.29	B	C
ATOM	7005	CE3	TRP	157	114.658	77.928	35.046	1.00	21.12	B	C
ATOM	7006	CD1	TRP	157	113.621	75.460	37.492	1.00	22.04	B	C

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## FIG. 4 - 144

(Continued)

ATOM	7007	NE1	TRP	157	113.193	76.650	38.030	1.00	22.01	B	N
ATOM	7008	CZ2	TRP	157	113.317	79.051	37.286	1.00	22.77	B	C
ATOM	7009	CZ3	TRP	157	114.445	79.299	35.156	1.00	22.58	B	C
ATOM	7010	CH2	TRP	157	113.779	79.846	36.270	1.00	21.74	B	C
ATOM	7011	C	TRP	157	115.096	73.640	33.153	1.00	22.79	B	C
ATOM	7012	O	TRP	157	114.789	72.483	32.882	1.00	23.16	B	O
ATOM	7013	N	SER	158	116.198	74.211	32.697	1.00	21.93	B	N
ATOM	7014	CA	SER	158	117.154	73.441	31.928	1.00	22.68	B	C
ATOM	7015	CB	SER	158	118.104	74.377	31.172	1.00	23.20	B	C
ATOM	7016	OG	SER	158	118.550	75.444	31.996	1.00	22.94	B	O
ATOM	7017	C	SER	158	117.898	72.667	33.017	1.00	23.12	B	C
ATOM	7018	O	SER	158	117.800	73.006	34.198	1.00	23.58	B	O
ATOM	7019	N	PRO	159	118.641	71.619	32.650	1.00	23.10	B	N
ATOM	7020	CD	PRO	159	118.927	71.096	31.307	1.00	23.69	B	C
ATOM	7021	CA	PRO	159	119.362	70.860	33.679	1.00	24.10	B	C
ATOM	7022	CB	PRO	159	120.041	69.744	32.886	1.00	24.45	B	C
ATOM	7023	CG	PRO	159	119.230	69.660	31.599	1.00	23.97	B	C
ATOM	7024	C	PRO	159	120.384	71.738	34.391	1.00	25.41	B	C
ATOM	7025	O	PRO	159	120.598	71.619	35.589	1.00	26.39	B	O
ATOM	7026	N	VAL	160	121.014	72.619	33.627	1.00	27.71	B	N
ATOM	7027	CA	VAL	160	122.031	73.517	34.146	1.00	29.28	B	C
ATOM	7028	CB	VAL	160	123.383	73.272	33.438	1.00	30.65	B	C
ATOM	7029	CG1	VAL	160	124.421	74.249	33.939	1.00	33.70	B	C
ATOM	7030	CG2	VAL	160	123.844	71.840	33.670	1.00	31.96	B	C
ATOM	7031	C	VAL	160	121.606	74.952	33.885	1.00	29.74	B	C
ATOM	7032	O	VAL	160	120.889	75.224	32.923	1.00	30.93	B	O
ATOM	7033	N	GLY	161	122.043	75.866	34.745	1.00	29.32	B	N
ATOM	7034	CA	GLY	161	121.706	77.266	34.562	1.00	28.43	B	C
ATOM	7035	C	GLY	161	120.289	77.645	34.944	1.00	28.19	B	C
ATOM	7036	O	GLY	161	119.839	77.359	36.053	1.00	30.02	B	O
ATOM	7037	N	HIS	162	119.584	78.296	34.025	1.00	26.53	B	N
ATOM	7038	CA	HIS	162	118.222	78.721	34.290	1.00	25.12	B	C
ATOM	7039	CB	HIS	162	118.214	79.959	35.177	1.00	26.70	B	C
ATOM	7040	CG	HIS	162	119.019	81.094	34.629	1.00	29.24	B	C
ATOM	7041	CD2	HIS	162	118.664	82.148	33.857	1.00	30.20	B	C
ATOM	7042	ND1	HIS	162	120.378	81.208	34.830	1.00	29.95	B	N
ATOM	7043	CE1	HIS	162	120.824	82.283	34.207	1.00	30.75	B	C
ATOM	7044	NE2	HIS	162	119.804	82.871	33.608	1.00	30.77	B	N
ATOM	7045	C	HIS	162	117.384	79.021	33.059	1.00	24.68	B	C
ATOM	7046	O	HIS	162	116.730	80.061	33.007	1.00	24.17	B	O
ATOM	7047	N	LYS	163	117.406	78.135	32.067	1.00	22.79	B	N
ATOM	7048	CA	LYS	163	116.575	78.340	30.889	1.00	23.10	B	C
ATOM	7049	CB	LYS	163	117.113	77.578	29.675	1.00	22.90	B	C
ATOM	7050	CG	LYS	163	118.367	78.184	29.063	1.00	23.40	B	C
ATOM	7051	CD	LYS	163	118.797	77.407	27.841	1.00	22.69	B	C
ATOM	7052	CE	LYS	163	120.103	77.930	27.282	1.00	23.67	B	C
ATOM	7053	NZ	LYS	163	120.616	77.045	26.195	1.00	24.56	B	N
ATOM	7054	C	LYS	163	115.215	77.779	31.266	1.00	24.15	B	C
ATOM	7055	O	LYS	163	115.079	77.104	32.282	1.00	24.69	B	O

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## FIG. 4 - 145

(Continued)

ATOM	7056	N	LEU	164	114.210	78.062	30.450	1.00	24.82	B	N
ATOM	7057	CA	LEU	164	112.870	77.572	30.704	1.00	24.27	B	C
ATOM	7058	CB	LEU	164	111.991	78.672	31.293	1.00	25.27	B	C
ATOM	7059	CG	LEU	164	112.216	78.969	32.769	1.00	25.61	B	C
ATOM	7060	CD1	LEU	164	111.420	80.181	33.178	1.00	25.08	B	C
ATOM	7061	CD2	LEU	164	111.802	77.756	33.582	1.00	28.15	B	C
ATOM	7062	C	LEU	164	112.231	77.068	29.435	1.00	25.20	B	C
ATOM	7063	O	LEU	164	112.438	77.616	28.353	1.00	26.77	B	O
ATOM	7064	N	ALA	165	111.461	76.003	29.581	1.00	24.98	B	N
ATOM	7065	CA	ALA	165	110.736	75.408	28.479	1.00	23.92	B	C
ATOM	7066	CB	ALA	165	111.408	74.127	28.021	1.00	23.20	B	C
ATOM	7067	C	ALA	165	109.394	75.106	29.114	1.00	25.13	B	C
ATOM	7068	O	ALA	165	109.326	74.494	30.188	1.00	24.88	B	O
ATOM	7069	N	TYR	166	108.326	75.565	28.481	1.00	24.06	B	N
ATOM	7070	CA	TYR	166	107.016	75.317	29.027	1.00	24.24	B	C
ATOM	7071	CB	TYR	166	106.556	76.522	29.866	1.00	27.58	B	C
ATOM	7072	CG	TYR	166	106.370	77.826	29.115	1.00	30.69	B	C
ATOM	7073	CD1	TYR	166	105.171	78.115	28.465	1.00	31.46	B	C
ATOM	7074	CE1	TYR	166	104.981	79.329	27.800	1.00	32.97	B	C
ATOM	7075	CD2	TYR	166	107.386	78.787	29.077	1.00	33.05	B	C
ATOM	7076	CE2	TYR	166	107.210	80.005	28.412	1.00	34.06	B	C
ATOM	7077	CZ	TYR	166	105.999	80.270	27.779	1.00	34.75	B	C
ATOM	7078	OH	TYR	166	105.789	81.485	27.162	1.00	34.83	B	O
ATOM	7079	C	TYR	166	106.039	75.003	27.917	1.00	23.86	B	C
ATOM	7080	O	TYR	166	106.276	75.333	26.754	1.00	22.73	B	O
ATOM	7081	N	VAL	167	104.955	74.321	28.266	1.00	22.73	B	N
ATOM	7082	CA	VAL	167	103.960	73.994	27.269	1.00	22.82	B	C
ATOM	7083	CB	VAL	167	103.687	72.487	27.215	1.00	21.03	B	C
ATOM	7084	CG1	VAL	167	102.528	72.200	26.274	1.00	17.71	B	C
ATOM	7085	CG2	VAL	167	104.933	71.770	26.725	1.00	20.37	B	C
ATOM	7086	C	VAL	167	102.683	74.754	27.564	1.00	23.41	B	C
ATOM	7087	O	VAL	167	102.196	74.779	28.692	1.00	24.72	B	O
ATOM	7088	N	TRP	168	102.162	75.394	26.531	1.00	23.89	B	N
ATOM	7089	CA	TRP	168	100.948	76.179	26.647	1.00	24.11	B	C
ATOM	7090	CB	TRP	168	101.314	77.664	26.655	1.00	24.80	B	C
ATOM	7091	CG	TRP	168	100.171	78.550	26.958	1.00	27.20	B	C
ATOM	7092	CD2	TRP	168	99.572	79.499	26.075	1.00	26.49	B	C
ATOM	7093	CE2	TRP	168	98.496	80.091	26.769	1.00	27.49	B	C
ATOM	7094	CE3	TRP	168	99.839	79.907	24.763	1.00	27.63	B	C
ATOM	7095	CD1	TRP	168	99.461	78.602	28.122	1.00	27.14	B	C
ATOM	7096	NE1	TRP	168	98.452	79.526	28.017	1.00	27.81	B	N
ATOM	7097	CZ2	TRP	168	97.682	81.074	26.194	1.00	26.74	B	C
ATOM	7098	CZ3	TRP	168	99.029	80.886	24.189	1.00	29.25	B	C
ATOM	7099	CH2	TRP	168	97.962	81.456	24.910	1.00	28.86	B	C
ATOM	7100	C	TRP	168	100.072	75.838	25.444	1.00	22.93	B	C
ATOM	7101	O	TRP	168	100.577	75.692	24.328	1.00	21.98	B	O
ATOM	7102	N	ASN	169	98.768	75.705	25.675	1.00	21.44	B	N
ATOM	7103	CA	ASN	169	97.830	75.350	24.610	1.00	22.01	B	C
ATOM	7104	CB	ASN	169	97.394	76.580	23.813	1.00	23.30	B	C

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## FIG. 4 - 146

(Continued)

ATOM	7105	CG	ASN	169	96.682	77.615	24.662	1.00	27.95	B	C
ATOM	7106	OD1	ASN	169	96.240	78.640	24.150	1.00	32.66	B	O
ATOM	7107	ND2	ASN	169	96.570	77.361	25.961	1.00	30.33	B	N
ATOM	7108	C	ASN	169	98.463	74.345	23.655	1.00	21.23	B	C
ATOM	7109	O	ASN	169	98.455	74.541	22.441	1.00	22.01	B	O
ATOM	7110	N	ASN	170	99.031	73.283	24.221	1.00	20.60	B	N
ATOM	7111	CA	ASN	170	99.661	72.208	23.459	1.00	20.97	B	C
ATOM	7112	CB	ASN	170	98.615	71.515	22.592	1.00	18.68	B	C
ATOM	7113	CG	ASN	170	97.629	70.741	23.412	1.00	18.15	B	C
ATOM	7114	OD1	ASN	170	97.158	71.224	24.440	1.00	16.27	B	O
ATOM	7115	ND2	ASN	170	97.300	69.529	22.966	1.00	18.92	B	N
ATOM	7116	C	ASN	170	100.859	72.581	22.598	1.00	21.31	B	C
ATOM	7117	O	ASN	170	101.194	71.861	21.659	1.00	20.36	B	O
ATOM	7118	N	ASP	171	101.504	73.697	22.916	1.00	22.16	B	N
ATOM	7119	CA	ASP	171	102.671	74.122	22.160	1.00	23.35	B	C
ATOM	7120	CB	ASP	171	102.354	75.364	21.334	1.00	23.05	B	C
ATOM	7121	CG	ASP	171	101.794	75.017	19.978	1.00	23.72	B	C
ATOM	7122	OD1	ASP	171	102.505	74.338	19.210	1.00	23.33	B	O
ATOM	7123	OD2	ASP	171	100.650	75.415	19.679	1.00	26.97	B	O
ATOM	7124	C	ASP	171	103.850	74.380	23.073	1.00	23.59	B	C
ATOM	7125	O	ASP	171	103.672	74.647	24.264	1.00	24.18	B	O
ATOM	7126	N	ILE	172	105.051	74.301	22.508	1.00	23.60	B	N
ATOM	7127	CA	ILE	172	106.273	74.497	23.281	1.00	25.23	B	C
ATOM	7128	CB	ILE	172	107.353	73.456	22.885	1.00	23.64	B	C
ATOM	7129	CG2	ILE	172	108.480	73.466	23.896	1.00	23.11	B	C
ATOM	7130	CG1	ILE	172	106.743	72.056	22.846	1.00	23.95	B	C
ATOM	7131	CD1	ILE	172	107.707	70.986	22.374	1.00	23.66	B	C
ATOM	7132	C	ILE	172	106.878	75.892	23.129	1.00	25.59	B	C
ATOM	7133	O	ILE	172	106.881	76.474	22.048	1.00	25.83	B	O
ATOM	7134	N	TYR	173	107.389	76.414	24.236	1.00	26.85	B	N
ATOM	7135	CA	TYR	173	108.025	77.720	24.272	1.00	27.95	B	C
ATOM	7136	CB	TYR	173	107.111	78.760	24.933	1.00	27.81	B	C
ATOM	7137	CG	TYR	173	105.822	79.002	24.190	1.00	29.53	B	C
ATOM	7138	CD1	TYR	173	104.788	78.063	24.226	1.00	29.72	B	C
ATOM	7139	CE1	TYR	173	103.599	78.271	23.535	1.00	29.08	B	C
ATOM	7140	CD2	TYR	173	105.634	80.162	23.439	1.00	28.71	B	C
ATOM	7141	CE2	TYR	173	104.444	80.381	22.740	1.00	30.14	B	C
ATOM	7142	CZ	TYR	173	103.432	79.429	22.794	1.00	30.82	B	C
ATOM	7143	OH	TYR	173	102.258	79.625	22.103	1.00	31.14	B	O
ATOM	7144	C	TYR	173	109.308	77.592	25.080	1.00	28.66	B	C
ATOM	7145	O	TYR	173	109.412	76.735	25.960	1.00	28.10	B	O
ATOM	7146	N	VAL	174	110.276	78.451	24.782	1.00	29.35	B	N
ATOM	7147	CA	VAL	174	111.551	78.443	25.480	1.00	29.22	B	C
ATOM	7148	CB	VAL	174	112.669	77.855	24.587	1.00	29.66	B	C
ATOM	7149	CG1	VAL	174	114.006	77.936	25.303	1.00	30.07	B	C
ATOM	7150	CG2	VAL	174	112.351	76.403	24.231	1.00	30.25	B	C
ATOM	7151	C	VAL	174	111.953	79.857	25.887	1.00	30.16	B	C
ATOM	7152	O	VAL	174	111.787	80.804	25.125	1.00	31.81	B	O
ATOM	7153	N	LYS	175	112.474	79.990	27.099	1.00	29.78	B	N

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## FIG. 4 - 147

(Continued)

ATOM	7154	CA	LYS	175	112.940	81.269	27.608	1.00	28.47	B	C
ATOM	7155	CB	LYS	175	112.090	81.725	28.794	1.00	28.38	B	C
ATOM	7156	CG	LYS	175	110.809	82.428	28.413	1.00	29.46	B	C
ATOM	7157	CD	LYS	175	109.876	82.551	29.611	1.00	32.27	B	C
ATOM	7158	CE	LYS	175	110.479	83.384	30.725	1.00	31.57	B	C
ATOM	7159	NZ	LYS	175	110.664	84.791	30.307	1.00	33.57	B	N
ATOM	7160	C	LYS	175	114.382	81.107	28.064	1.00	28.80	B	C
ATOM	7161	O	LYS	175	114.662	80.355	28.999	1.00	28.36	B	O
ATOM	7162	N	ILE	176	115.294	81.813	27.401	1.00	28.58	B	N
ATOM	7163	CA	ILE	176	116.710	81.764	27.749	1.00	28.19	B	C
ATOM	7164	CB	ILE	176	117.572	82.363	26.624	1.00	27.21	B	C
ATOM	7165	CG2	ILE	176	118.942	82.730	27.146	1.00	25.54	B	C
ATOM	7166	CG1	ILE	176	117.697	81.354	25.483	1.00	28.29	B	C
ATOM	7167	CD1	ILE	176	116.377	80.941	24.861	1.00	27.38	B	C
ATOM	7168	C	ILE	176	116.956	82.528	29.044	1.00	29.36	B	C
ATOM	7169	O	ILE	176	117.910	82.251	29.768	1.00	29.16	B	O
ATOM	7170	N	GLU	177	116.085	83.489	29.330	1.00	31.44	B	N
ATOM	7171	CA	GLU	177	116.182	84.296	30.543	1.00	33.96	B	C
ATOM	7172	CB	GLU	177	116.901	85.611	30.241	1.00	35.87	B	C
ATOM	7173	CG	GLU	177	118.342	85.440	29.770	1.00	37.59	B	C
ATOM	7174	CD	GLU	177	119.324	85.272	30.916	1.00	39.82	B	C
ATOM	7175	OE1	GLU	177	120.511	84.988	30.642	1.00	40.62	B	O
ATOM	7176	OE2	GLU	177	118.914	85.433	32.088	1.00	40.43	B	O
ATOM	7177	C	GLU	177	114.762	84.569	31.034	1.00	34.61	B	C
ATOM	7178	O	GLU	177	113.905	85.007	30.268	1.00	35.24	B	O
ATOM	7179	N	PRO	178	114.495	84.312	32.323	1.00	35.55	B	N
ATOM	7180	CD	PRO	178	115.451	83.907	33.367	1.00	36.07	B	C
ATOM	7181	CA	PRO	178	113.160	84.530	32.894	1.00	35.46	B	C
ATOM	7182	CB	PRO	178	113.383	84.357	34.402	1.00	35.40	B	C
ATOM	7183	CG	PRO	178	114.862	84.563	34.587	1.00	37.12	B	C
ATOM	7184	C	PRO	178	112.451	85.834	32.547	1.00	35.74	B	C
ATOM	7185	O	PRO	178	111.225	85.859	32.446	1.00	35.44	B	O
ATOM	7186	N	ASN	179	113.198	86.912	32.346	1.00	36.89	B	N
ATOM	7187	CA	ASN	179	112.560	88.188	32.021	1.00	37.31	B	C
ATOM	7188	CB	ASN	179	113.211	89.329	32.807	1.00	37.54	B	C
ATOM	7189	CG	ASN	179	114.454	89.860	32.137	1.00	37.86	B	C
ATOM	7190	OD1	ASN	179	115.419	89.131	31.915	1.00	39.14	B	O
ATOM	7191	ND2	ASN	179	114.437	91.142	31.806	1.00	40.48	B	N
ATOM	7192	C	ASN	179	112.573	88.540	30.535	1.00	36.88	B	C
ATOM	7193	O	ASN	179	112.205	89.650	30.159	1.00	38.11	B	O
ATOM	7194	N	LEU	180	112.995	87.608	29.689	1.00	35.31	B	N
ATOM	7195	CA	LEU	180	113.030	87.875	28.260	1.00	34.44	B	C
ATOM	7196	CB	LEU	180	114.357	87.417	27.662	1.00	35.92	B	C
ATOM	7197	CG	LEU	180	115.621	88.014	28.279	1.00	36.91	B	C
ATOM	7198	CD1	LEU	180	116.828	87.572	27.470	1.00	37.09	B	C
ATOM	7199	CD2	LEU	180	115.522	89.536	28.303	1.00	37.24	B	C
ATOM	7200	C	LEU	180	111.898	87.166	27.547	1.00	33.52	B	C
ATOM	7201	O	LEU	180	111.406	86.149	28.015	1.00	32.50	B	O
ATOM	7202	N	PRO	181	111.462	87.704	26.400	1.00	34.20	B	N

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## FIG. 4 - 148

(Continued)

ATOM	7203	CD	PRO	181	111.853	88.984	25.784	1.00	33.21	B	C
ATOM	7204	CA	PRO	181	110.373	87.075	25.645	1.00	33.57	B	C
ATOM	7205	CB	PRO	181	110.337	87.890	24.357	1.00	33.27	B	C
ATOM	7206	CG	PRO	181	110.691	89.259	24.846	1.00	33.21	B	C
ATOM	7207	C	PRO	181	110.681	85.608	25.397	1.00	33.03	B	C
ATOM	7208	O	PRO	181	111.829	85.180	25.497	1.00	33.18	B	O
ATOM	7209	N	SER	182	109.654	84.838	25.070	1.00	33.87	B	N
ATOM	7210	CA	SER	182	109.835	83.415	24.829	1.00	32.06	B	C
ATOM	7211	CB	SER	182	108.752	82.622	25.547	1.00	31.33	B	C
ATOM	7212	OG	SER	182	107.505	82.817	24.909	1.00	30.50	B	O
ATOM	7213	C	SER	182	109.759	83.117	23.350	1.00	31.89	B	C
ATOM	7214	O	SER	182	109.077	83.812	22.606	1.00	33.14	B	O
ATOM	7215	N	TYR	183	110.463	82.077	22.927	1.00	31.53	B	N
ATOM	7216	CA	TYR	183	110.453	81.677	21.532	1.00	30.47	B	C
ATOM	7217	CB	TYR	183	111.832	81.159	21.118	1.00	30.68	B	C
ATOM	7218	CG	TYR	183	112.962	82.117	21.408	1.00	32.75	B	C
ATOM	7219	CD1	TYR	183	113.490	82.235	22.696	1.00	32.39	B	C
ATOM	7220	CE1	TYR	183	114.517	83.134	22.977	1.00	33.30	B	C
ATOM	7221	CD2	TYR	183	113.492	82.926	20.398	1.00	33.06	B	C
ATOM	7222	CE2	TYR	183	114.520	83.832	20.667	1.00	34.20	B	C
ATOM	7223	CZ	TYR	183	115.028	83.932	21.959	1.00	34.92	B	C
ATOM	7224	OH	TYR	183	116.036	84.832	22.233	1.00	34.60	B	O
ATOM	7225	C	TYR	183	109.423	80.568	21.384	1.00	29.28	B	C
ATOM	7226	O	TYR	183	109.387	79.645	22.196	1.00	29.66	B	O
ATOM	7227	N	ARG	184	108.579	80.659	20.364	1.00	27.67	B	N
ATOM	7228	CA	ARG	184	107.573	79.631	20.148	1.00	26.57	B	C
ATOM	7229	CB	ARG	184	106.327	80.217	19.476	1.00	26.06	B	C
ATOM	7230	CG	ARG	184	105.215	79.191	19.285	1.00	28.64	B	C
ATOM	7231	CD	ARG	184	103.860	79.825	19.004	1.00	30.29	B	C
ATOM	7232	NE	ARG	184	102.827	78.805	18.831	1.00	31.47	B	N
ATOM	7233	CZ	ARG	184	101.526	79.052	18.706	1.00	29.99	B	C
ATOM	7234	NH1	ARG	184	100.678	78.048	18.552	1.00	30.76	B	N
ATOM	7235	NH2	ARG	184	101.068	80.294	18.740	1.00	30.05	B	N
ATOM	7236	C	ARG	184	108.185	78.553	19.272	1.00	26.51	B	C
ATOM	7237	O	ARG	184	108.375	78.754	18.072	1.00	28.42	B	O
ATOM	7238	N	ILE	185	108.493	77.411	19.876	1.00	24.50	B	N
ATOM	7239	CA	ILE	185	109.112	76.303	19.165	1.00	22.88	B	C
ATOM	7240	CB	ILE	185	109.773	75.319	20.159	1.00	23.12	B	C
ATOM	7241	CG2	ILE	185	110.492	74.216	19.405	1.00	22.56	B	C
ATOM	7242	CG1	ILE	185	110.753	76.067	21.064	1.00	22.32	B	C
ATOM	7243	CD1	ILE	185	111.869	76.770	20.324	1.00	21.93	B	C
ATOM	7244	C	ILE	185	108.148	75.516	18.275	1.00	24.00	B	C
ATOM	7245	O	ILE	185	108.569	74.930	17.275	1.00	25.07	B	O
ATOM	7246	N	THR	186	106.866	75.489	18.632	1.00	22.70	B	N
ATOM	7247	CA	THR	186	105.886	74.750	17.840	1.00	23.30	B	C
ATOM	7248	CB	THR	186	105.490	73.440	18.541	1.00	22.83	B	C
ATOM	7249	OG1	THR	186	105.058	73.727	19.877	1.00	27.42	B	O
ATOM	7250	CG2	THR	186	106.665	72.491	18.595	1.00	19.86	B	C
ATOM	7251	C	THR	186	104.620	75.548	17.537	1.00	23.45	B	C

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## FIG. 4 - 149

(Continued)

ATOM	7252	O	THR	186	104.266	76.469	18.265	1.00	22.05	B	O
ATOM	7253	N	TRP	187	103.935	75.179	16.457	1.00	24.88	B	N
ATOM	7254	CA	TRP	187	102.717	75.876	16.049	1.00	25.32	B	C
ATOM	7255	CB	TRP	187	103.007	76.767	14.832	1.00	25.43	B	C
ATOM	7256	CG	TRP	187	104.159	77.694	15.025	1.00	25.95	B	C
ATOM	7257	CD2	TRP	187	104.093	79.092	15.321	1.00	26.73	B	C
ATOM	7258	CE2	TRP	187	105.420	79.548	15.487	1.00	26.07	B	C
ATOM	7259	CE3	TRP	187	103.041	80.007	15.464	1.00	27.09	B	C
ATOM	7260	CD1	TRP	187	105.485	77.367	15.019	1.00	26.93	B	C
ATOM	7261	NE1	TRP	187	106.249	78.474	15.298	1.00	26.08	B	N
ATOM	7262	CZ2	TRP	187	105.723	80.878	15.789	1.00	24.50	B	C
ATOM	7263	CZ3	TRP	187	103.346	81.332	15.764	1.00	26.71	B	C
ATOM	7264	CH2	TRP	187	104.679	81.751	15.922	1.00	25.13	B	C
ATOM	7265	C	TRP	187	101.555	74.941	15.709	1.00	26.00	B	C
ATOM	7266	O	TRP	187	100.481	75.402	15.339	1.00	27.74	B	O
ATOM	7267	N	THR	188	101.759	73.636	15.839	1.00	26.58	B	N
ATOM	7268	CA	THR	188	100.708	72.672	15.516	1.00	26.89	B	C
ATOM	7269	CB	THR	188	101.304	71.388	14.895	1.00	26.63	B	C
ATOM	7270	OG1	THR	188	102.291	70.836	15.781	1.00	27.13	B	O
ATOM	7271	CG2	THR	188	101.940	71.697	13.552	1.00	25.34	B	C
ATOM	7272	C	THR	188	99.817	72.259	16.687	1.00	27.17	B	C
ATOM	7273	O	THR	188	98.916	71.437	16.512	1.00	26.92	B	O
ATOM	7274	N	GLY	189	100.064	72.827	17.866	1.00	26.58	B	N
ATOM	7275	CA	GLY	189	99.278	72.491	19.045	1.00	27.32	B	C
ATOM	7276	C	GLY	189	97.783	72.645	18.847	1.00	28.44	B	C
ATOM	7277	O	GLY	189	97.333	73.673	18.345	1.00	30.95	B	O
ATOM	7278	N	LYS	190	97.007	71.636	19.242	1.00	27.83	B	N
ATOM	7279	CA	LYS	190	95.554	71.686	19.085	1.00	27.15	B	C
ATOM	7280	CB	LYS	190	95.187	71.381	17.628	1.00	29.55	B	C
ATOM	7281	CG	LYS	190	93.695	71.294	17.317	1.00	31.55	B	C
ATOM	7282	CD	LYS	190	93.498	71.031	15.821	1.00	36.65	B	C
ATOM	7283	CE	LYS	190	92.043	70.731	15.458	1.00	39.17	B	C
ATOM	7284	NZ	LYS	190	91.127	71.870	15.744	1.00	41.50	B	N
ATOM	7285	C	LYS	190	94.815	70.731	20.028	1.00	26.61	B	C
ATOM	7286	O	LYS	190	94.738	69.523	19.786	1.00	25.87	B	O
ATOM	7287	N	GLU	191	94.262	71.299	21.096	1.00	25.05	B	N
ATOM	7288	CA	GLU	191	93.516	70.558	22.110	1.00	25.10	B	C
ATOM	7289	CB	GLU	191	92.461	71.475	22.728	1.00	26.71	B	C
ATOM	7290	CG	GLU	191	91.821	70.933	23.987	1.00	29.36	B	C
ATOM	7291	CD	GLU	191	90.752	71.859	24.514	1.00	34.15	B	C
ATOM	7292	OE1	GLU	191	90.111	71.522	25.536	1.00	36.46	B	O
ATOM	7293	OE2	GLU	191	90.551	72.932	23.899	1.00	35.96	B	O
ATOM	7294	C	GLU	191	92.849	69.263	21.631	1.00	23.31	B	C
ATOM	7295	O	GLU	191	92.031	69.280	20.713	1.00	20.17	B	O
ATOM	7296	N	ASP	192	93.208	68.157	22.287	1.00	23.70	B	N
ATOM	7297	CA	ASP	192	92.707	66.811	21.996	1.00	24.98	B	C
ATOM	7298	CB	ASP	192	91.183	66.733	22.149	1.00	27.27	B	C
ATOM	7299	CG	ASP	192	90.700	67.200	23.508	1.00	30.85	B	C
ATOM	7300	OD1	ASP	192	91.335	66.855	24.533	1.00	32.45	B	O

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## FIG. 4 - 150

(Continued)

ATOM	7301	OD2	ASP	192	89.671	67.908	23.548	1.00	32.44	B	O
ATOM	7302	C	ASP	192	93.072	66.329	20.602	1.00	25.95	B	C
ATOM	7303	O	ASP	192	92.431	65.426	20.065	1.00	27.81	B	O
ATOM	7304	N	ILE	193	94.091	66.926	20.000	1.00	25.46	B	N
ATOM	7305	CA	ILE	193	94.485	66.512	18.665	1.00	25.50	B	C
ATOM	7306	CB	ILE	193	93.970	67.502	17.595	1.00	26.97	B	C
ATOM	7307	CG2	ILE	193	94.426	67.057	16.212	1.00	26.11	B	C
ATOM	7308	CG1	ILE	193	92.441	67.552	17.621	1.00	27.90	B	C
ATOM	7309	CD1	ILE	193	91.784	66.246	17.210	1.00	29.23	B	C
ATOM	7310	C	ILE	193	95.994	66.390	18.546	1.00	25.04	B	C
ATOM	7311	O	ILE	193	96.519	65.297	18.334	1.00	26.34	B	O
ATOM	7312	N	ILE	194	96.691	67.510	18.682	1.00	22.43	B	N
ATOM	7313	CA	ILE	194	98.139	67.505	18.589	1.00	21.47	B	C
ATOM	7314	CB	ILE	194	98.618	68.429	17.456	1.00	21.58	B	C
ATOM	7315	CG2	ILE	194	100.146	68.414	17.377	1.00	18.60	B	C
ATOM	7316	CG1	ILE	194	97.972	68.001	16.133	1.00	19.45	B	C
ATOM	7317	CD1	ILE	194	98.331	66.613	15.678	1.00	15.81	B	C
ATOM	7318	C	ILE	194	98.779	67.968	19.895	1.00	21.61	B	C
ATOM	7319	O	ILE	194	98.544	69.095	20.337	1.00	22.13	B	O
ATOM	7320	N	TYR	195	99.580	67.095	20.508	1.00	19.09	B	N
ATOM	7321	CA	TYR	195	100.272	67.429	21.750	1.00	18.17	B	C
ATOM	7322	CB	TYR	195	100.079	66.331	22.798	1.00	20.45	B	C
ATOM	7323	CG	TYR	195	98.647	65.941	23.094	1.00	21.37	B	C
ATOM	7324	CD1	TYR	195	97.873	65.269	22.146	1.00	20.38	B	C
ATOM	7325	CE1	TYR	195	96.584	64.846	22.445	1.00	20.38	B	C
ATOM	7326	CD2	TYR	195	98.087	66.187	24.349	1.00	21.55	B	C
ATOM	7327	CE2	TYR	195	96.797	65.768	24.659	1.00	20.75	B	C
ATOM	7328	CZ	TYR	195	96.052	65.094	23.705	1.00	20.48	B	C
ATOM	7329	OH	TYR	195	94.785	64.650	24.020	1.00	19.77	B	O
ATOM	7330	C	TYR	195	101.771	67.579	21.503	1.00	18.27	B	C
ATOM	7331	O	TYR	195	102.412	66.677	20.967	1.00	19.50	B	O
ATOM	7332	N	ASN	196	102.334	68.710	21.897	1.00	17.52	B	N
ATOM	7333	CA	ASN	196	103.762	68.941	21.725	1.00	17.79	B	C
ATOM	7334	CB	ASN	196	104.011	70.187	20.867	1.00	17.21	B	C
ATOM	7335	CG	ASN	196	103.366	70.106	19.489	1.00	17.04	B	C
ATOM	7336	OD1	ASN	196	103.769	69.311	18.632	1.00	16.41	B	O
ATOM	7337	ND2	ASN	196	102.362	70.943	19.267	1.00	17.01	B	N
ATOM	7338	C	ASN	196	104.380	69.160	23.104	1.00	18.89	B	C
ATOM	7339	O	ASN	196	103.976	70.066	23.828	1.00	21.80	B	O
ATOM	7340	N	GLY	197	105.355	68.344	23.479	1.00	18.21	B	N
ATOM	7341	CA	GLY	197	105.976	68.533	24.778	1.00	18.42	B	C
ATOM	7342	C	GLY	197	105.185	67.948	25.941	1.00	18.43	B	C
ATOM	7343	O	GLY	197	105.660	67.954	27.088	1.00	17.86	B	O
ATOM	7344	N	ILE	198	103.976	67.469	25.654	1.00	15.16	B	N
ATOM	7345	CA	ILE	198	103.129	66.842	26.667	1.00	14.58	B	C
ATOM	7346	CB	ILE	198	101.956	67.740	27.160	1.00	12.66	B	C
ATOM	7347	CG2	ILE	198	102.477	68.784	28.109	1.00	10.73	B	C
ATOM	7348	CG1	ILE	198	101.189	68.334	25.970	1.00	14.13	B	C
ATOM	7349	CD1	ILE	198	99.936	69.129	26.368	1.00	13.46	B	C

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## FIG. 4 - 151

(Continued)

ATOM	7350	C	ILE	198	102.523	65.585	26.101	1.00	14.46	B	C
ATOM	7351	O	ILE	198	102.354	65.447	24.895	1.00	16.78	B	O
ATOM	7352	N	THR	199	102.182	64.671	26.990	1.00	15.77	B	N
ATOM	7353	CA	THR	199	101.600	63.396	26.608	1.00	15.94	B	C
ATOM	7354	CB	THR	199	101.982	62.350	27.630	1.00	15.69	B	C
ATOM	7355	OG1	THR	199	101.683	62.861	28.937	1.00	12.99	B	O
ATOM	7356	CG2	THR	199	103.473	62.043	27.534	1.00	15.54	B	C
ATOM	7357	C	THR	199	100.085	63.448	26.522	1.00	15.87	B	C
ATOM	7358	O	THR	199	99.452	64.311	27.133	1.00	16.77	B	O
ATOM	7359	N	ASP	200	99.510	62.534	25.745	1.00	16.29	B	N
ATOM	7360	CA	ASP	200	98.058	62.450	25.619	1.00	16.42	B	C
ATOM	7361	CB	ASP	200	97.654	61.812	24.279	1.00	17.56	B	C
ATOM	7362	CG	ASP	200	97.960	60.321	24.207	1.00	19.40	B	C
ATOM	7363	OD1	ASP	200	98.894	59.847	24.892	1.00	20.07	B	O
ATOM	7364	OD2	ASP	200	97.267	59.624	23.438	1.00	19.79	B	O
ATOM	7365	C	ASP	200	97.657	61.578	26.806	1.00	15.56	B	C
ATOM	7366	O	ASP	200	98.502	61.278	27.648	1.00	16.67	B	O
ATOM	7367	N	TRP	201	96.404	61.151	26.889	1.00	14.09	B	N
ATOM	7368	CA	TRP	201	96.003	60.368	28.049	1.00	13.08	B	C
ATOM	7369	CB	TRP	201	94.503	60.106	28.037	1.00	13.25	B	C
ATOM	7370	CG	TRP	201	94.023	59.554	29.348	1.00	12.63	B	C
ATOM	7371	CD2	TRP	201	94.135	58.198	29.801	1.00	10.35	B	C
ATOM	7372	CE2	TRP	201	93.610	58.150	31.110	1.00	11.08	B	C
ATOM	7373	CE3	TRP	201	94.634	57.020	29.228	1.00	8.52	B	C
ATOM	7374	CD1	TRP	201	93.449	60.253	30.370	1.00	12.43	B	C
ATOM	7375	NE1	TRP	201	93.198	59.416	31.434	1.00	12.21	B	N
ATOM	7376	CZ2	TRP	201	93.567	56.967	31.858	1.00	11.85	B	C
ATOM	7377	CZ3	TRP	201	94.596	55.847	29.968	1.00	8.91	B	C
ATOM	7378	CH2	TRP	201	94.065	55.829	31.271	1.00	10.19	B	C
ATOM	7379	C	TRP	201	96.719	59.040	28.264	1.00	14.63	B	C
ATOM	7380	O	TRP	201	97.197	58.766	29.366	1.00	14.84	B	O
ATOM	7381	N	VAL	202	96.795	58.213	27.224	1.00	14.84	B	N
ATOM	7382	CA	VAL	202	97.413	56.902	27.369	1.00	13.74	B	C
ATOM	7383	CB	VAL	202	97.028	55.966	26.190	1.00	11.30	B	C
ATOM	7384	CG1	VAL	202	97.960	56.155	25.010	1.00	8.57	B	C
ATOM	7385	CG2	VAL	202	97.028	54.541	26.667	1.00	8.82	B	C
ATOM	7386	C	VAL	202	98.929	56.920	27.556	1.00	15.45	B	C
ATOM	7387	O	VAL	202	99.471	56.095	28.292	1.00	16.05	B	O
ATOM	7388	N	TYR	203	99.616	57.857	26.906	1.00	15.45	B	N
ATOM	7389	CA	TYR	203	101.060	57.941	27.053	1.00	13.39	B	C
ATOM	7390	CB	TYR	203	101.656	58.918	26.035	1.00	12.37	B	C
ATOM	7391	CG	TYR	203	102.248	58.238	24.823	1.00	8.90	B	C
ATOM	7392	CD1	TYR	203	101.461	57.938	23.709	1.00	8.82	B	C
ATOM	7393	CE1	TYR	203	101.989	57.260	22.619	1.00	7.48	B	C
ATOM	7394	CD2	TYR	203	103.587	57.844	24.812	1.00	5.53	B	C
ATOM	7395	CE2	TYR	203	104.128	57.167	23.727	1.00	6.51	B	C
ATOM	7396	CZ	TYR	203	103.325	56.874	22.634	1.00	8.49	B	C
ATOM	7397	OH	TYR	203	103.849	56.175	21.572	1.00	8.01	B	O
ATOM	7398	C	TYR	203	101.438	58.371	28.471	1.00	13.68	B	C

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(Continued)

## FIG. 4 - 152

ATOM	7399	O	TYR	203	102.369	57.832	29.056	1.00	12.65	B	O
ATOM	7400	N	GLU	204	100.706	59.335	29.020	1.00	15.26	B	N
ATOM	7401	CA	GLU	204	100.963	59.827	30.376	1.00	16.69	B	C
ATOM	7402	CB	GLU	204	99.975	60.936	30.743	1.00	16.67	B	C
ATOM	7403	CG	GLU	204	100.174	61.457	32.161	1.00	17.47	B	C
ATOM	7404	CD	GLU	204	98.950	62.154	32.731	1.00	17.71	B	C
ATOM	7405	OE1	GLU	204	98.197	62.785	31.964	1.00	19.00	B	O
ATOM	7406	OE2	GLU	204	98.753	62.085	33.962	1.00	18.59	B	O
ATOM	7407	C	GLU	204	100.831	58.740	31.437	1.00	17.37	B	C
ATOM	7408	O	GLU	204	101.681	58.597	32.305	1.00	18.22	B	O
ATOM	7409	N	GLU	205	99.745	57.980	31.353	1.00	18.89	B	N
ATOM	7410	CA	GLU	205	99.442	56.932	32.315	1.00	19.55	B	C
ATOM	7411	CB	GLU	205	97.925	56.727	32.344	1.00	20.80	B	C
ATOM	7412	CG	GLU	205	97.453	55.436	32.995	1.00	23.74	B	C
ATOM	7413	CD	GLU	205	97.414	55.494	34.515	1.00	26.68	B	C
ATOM	7414	OE1	GLU	205	97.038	54.466	35.118	1.00	28.71	B	O
ATOM	7415	OE2	GLU	205	97.744	56.547	35.106	1.00	26.12	B	O
ATOM	7416	C	GLU	205	100.132	55.578	32.131	1.00	19.27	B	C
ATOM	7417	O	GLU	205	100.525	54.957	33.107	1.00	19.31	B	O
ATOM	7418	N	GLU	206	100.291	55.124	30.893	1.00	18.93	B	N
ATOM	7419	CA	GLU	206	100.876	53.808	30.660	1.00	18.63	B	C
ATOM	7420	CB	GLU	206	99.989	53.016	29.705	1.00	18.05	B	C
ATOM	7421	CG	GLU	206	98.535	52.921	30.139	1.00	20.39	B	C
ATOM	7422	CD	GLU	206	98.359	52.143	31.422	1.00	20.74	B	C
ATOM	7423	OE1	GLU	206	97.205	51.905	31.821	1.00	21.45	B	O
ATOM	7424	OE2	GLU	206	99.375	51.768	32.037	1.00	22.90	B	O
ATOM	7425	C	GLU	206	102.293	53.766	30.136	1.00	19.32	B	C
ATOM	7426	O	GLU	206	102.976	52.761	30.292	1.00	20.01	B	O
ATOM	7427	N	VAL	207	102.744	54.844	29.509	1.00	20.90	B	N
ATOM	7428	CA	VAL	207	104.092	54.855	28.968	1.00	20.95	B	C
ATOM	7429	CB	VAL	207	104.101	55.347	27.509	1.00	21.52	B	C
ATOM	7430	CG1	VAL	207	105.486	55.151	26.918	1.00	22.17	B	C
ATOM	7431	CG2	VAL	207	103.048	54.592	26.684	1.00	19.10	B	C
ATOM	7432	C	VAL	207	105.080	55.691	29.775	1.00	21.67	B	C
ATOM	7433	O	VAL	207	106.052	55.160	30.301	1.00	25.32	B	O
ATOM	7434	N	PHE	208	104.833	56.989	29.888	1.00	21.55	B	N
ATOM	7435	CA	PHE	208	105.743	57.870	30.611	1.00	21.33	B	C
ATOM	7436	CB	PHE	208	105.877	59.201	29.863	1.00	21.28	B	C
ATOM	7437	CG	PHE	208	106.571	59.083	28.536	1.00	21.92	B	C
ATOM	7438	CD1	PHE	208	107.890	58.649	28.464	1.00	20.63	B	C
ATOM	7439	CD2	PHE	208	105.893	59.373	27.353	1.00	22.58	B	C
ATOM	7440	CE1	PHE	208	108.525	58.499	27.230	1.00	22.52	B	C
ATOM	7441	CE2	PHE	208	106.521	59.225	26.109	1.00	22.24	B	C
ATOM	7442	CZ	PHE	208	107.837	58.787	26.048	1.00	22.76	B	C
ATOM	7443	C	PHE	208	105.444	58.168	32.082	1.00	21.89	B	C
ATOM	7444	O	PHE	208	106.298	58.727	32.768	1.00	23.07	B	O
ATOM	7445	N	SER	209	104.261	57.811	32.577	1.00	20.48	B	N
ATOM	7446	CA	SER	209	103.922	58.094	33.976	1.00	19.86	B	C
ATOM	7447	CB	SER	209	104.689	57.165	34.905	1.00	18.09	B	C

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(Continued)

## FIG. 4 - 153

ATOM	7448	OG	SER	209	104.383	55.820	34.601	1.00	21.42	B	O
ATOM	7449	C	SER	209	104.285	59.543	34.286	1.00	20.55	B	C
ATOM	7450	O	SER	209	104.780	59.877	35.367	1.00	19.53	B	O
ATOM	7451	N	ALA	210	104.031	60.394	33.302	1.00	20.69	B	N
ATOM	7452	CA	ALA	210	104.319	61.809	33.393	1.00	20.47	B	C
ATOM	7453	CB	ALA	210	105.809	62.044	33.228	1.00	20.63	B	C
ATOM	7454	C	ALA	210	103.545	62.492	32.275	1.00	20.53	B	C
ATOM	7455	O	ALA	210	103.042	61.835	31.367	1.00	19.81	B	O
ATOM	7456	N	TYR	211	103.461	63.813	32.354	1.00	21.78	B	N
ATOM	7457	CA	TYR	211	102.733	64.634	31.390	1.00	20.95	B	C
ATOM	7458	CB	TYR	211	101.944	65.681	32.175	1.00	18.35	B	C
ATOM	7459	CG	TYR	211	100.984	66.566	31.411	1.00	15.38	B	C
ATOM	7460	CD1	TYR	211	100.257	66.086	30.324	1.00	14.13	B	C
ATOM	7461	CE1	TYR	211	99.310	66.879	29.694	1.00	12.47	B	C
ATOM	7462	CD2	TYR	211	100.738	67.863	31.846	1.00	11.95	B	C
ATOM	7463	CE2	TYR	211	99.799	68.657	31.231	1.00	12.21	B	C
ATOM	7464	CZ	TYR	211	99.087	68.165	30.156	1.00	13.68	B	C
ATOM	7465	OH	TYR	211	98.158	68.977	29.550	1.00	12.73	B	O
ATOM	7466	C	TYR	211	103.781	65.283	30.508	1.00	22.11	B	C
ATOM	7467	O	TYR	211	103.512	65.742	29.406	1.00	23.55	B	O
ATOM	7468	N	SER	212	105.000	65.294	31.017	1.00	23.17	B	N
ATOM	7469	CA	SER	212	106.112	65.877	30.310	1.00	22.03	B	C
ATOM	7470	CB	SER	212	107.286	66.055	31.265	1.00	22.38	B	C
ATOM	7471	OG	SER	212	108.441	66.477	30.567	1.00	24.83	B	O
ATOM	7472	C	SER	212	106.547	65.017	29.141	1.00	22.20	B	C
ATOM	7473	O	SER	212	106.651	63.802	29.256	1.00	22.93	B	O
ATOM	7474	N	ALA	213	106.791	65.668	28.013	1.00	22.14	B	N
ATOM	7475	CA	ALA	213	107.267	65.011	26.812	1.00	19.72	B	C
ATOM	7476	CB	ALA	213	106.157	64.882	25.803	1.00	19.85	B	C
ATOM	7477	C	ALA	213	108.360	65.942	26.301	1.00	21.17	B	C
ATOM	7478	O	ALA	213	108.443	66.254	25.109	1.00	20.14	B	O
ATOM	7479	N	LEU	214	109.175	66.409	27.243	1.00	21.21	B	N
ATOM	7480	CA	LEU	214	110.298	67.295	26.961	1.00	22.06	B	C
ATOM	7481	CB	LEU	214	110.049	68.697	27.534	1.00	21.02	B	C
ATOM	7482	CG	LEU	214	108.958	69.546	26.878	1.00	20.19	B	C
ATOM	7483	CD1	LEU	214	108.840	70.872	27.603	1.00	21.72	B	C
ATOM	7484	CD2	LEU	214	109.292	69.779	25.426	1.00	22.01	B	C
ATOM	7485	C	LEU	214	111.528	66.688	27.615	1.00	22.30	B	C
ATOM	7486	O	LEU	214	111.442	66.131	28.703	1.00	25.61	B	O
ATOM	7487	N	TRP	215	112.674	66.795	26.957	1.00	21.71	B	N
ATOM	7488	CA	TRP	215	113.904	66.237	27.497	1.00	19.34	B	C
ATOM	7489	CB	TRP	215	114.112	64.833	26.942	1.00	18.71	B	C
ATOM	7490	CG	TRP	215	113.018	63.863	27.294	1.00	18.43	B	C
ATOM	7491	CD2	TRP	215	111.910	63.481	26.468	1.00	16.56	B	C
ATOM	7492	CE2	TRP	215	111.157	62.536	27.194	1.00	14.85	B	C
ATOM	7493	CE3	TRP	215	111.482	63.845	25.186	1.00	17.01	B	C
ATOM	7494	CD1	TRP	215	112.890	63.155	28.456	1.00	15.04	B	C
ATOM	7495	NE1	TRP	215	111.781	62.356	28.400	1.00	13.49	B	N
ATOM	7496	CZ2	TRP	215	109.996	61.949	26.682	1.00	14.75	B	C

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## FIG. 4 - 154

(Continued)

ATOM	7497	CZ3	TRP	215	110.326	63.257	24.675	1.00	15.48	B	C
ATOM	7498	CH2	TRP	215	109.599	62.320	25.425	1.00	15.57	B	C
ATOM	7499	C	TRP	215	115.110	67.096	27.149	1.00	20.78	B	C
ATOM	7500	O	TRP	215	115.625	67.034	26.028	1.00	20.20	B	O
ATOM	7501	N	TRP	216	115.566	67.897	28.108	1.00	20.97	B	N
ATOM	7502	CA	TRP	216	116.727	68.743	27.880	1.00	21.49	B	C
ATOM	7503	CB	TRP	216	116.958	69.705	29.048	1.00	22.15	B	C
ATOM	7504	CG	TRP	216	116.020	70.863	29.156	1.00	24.63	B	C
ATOM	7505	CD2	TRP	216	116.097	72.099	28.437	1.00	25.56	B	C
ATOM	7506	CE2	TRP	216	115.036	72.916	28.896	1.00	26.21	B	C
ATOM	7507	CE3	TRP	216	116.959	72.598	27.452	1.00	25.00	B	C
ATOM	7508	CD1	TRP	216	114.945	70.974	29.994	1.00	25.92	B	C
ATOM	7509	NE1	TRP	216	114.351	72.204	29.844	1.00	26.55	B	N
ATOM	7510	CZ2	TRP	216	114.815	74.209	28.401	1.00	24.93	B	C
ATOM	7511	CZ3	TRP	216	116.738	73.887	26.958	1.00	25.52	B	C
ATOM	7512	CH2	TRP	216	115.673	74.674	27.435	1.00	24.95	B	C
ATOM	7513	C	TRP	216	117.982	67.896	27.747	1.00	23.03	B	C
ATOM	7514	O	TRP	216	118.083	66.816	28.334	1.00	21.32	B	O
ATOM	7515	N	SER	217	118.941	68.398	26.975	1.00	25.91	B	N
ATOM	7516	CA	SER	217	120.222	67.723	26.819	1.00	26.96	B	C
ATOM	7517	CB	SER	217	120.954	68.223	25.575	1.00	28.77	B	C
ATOM	7518	OG	SER	217	121.212	69.612	25.676	1.00	31.27	B	O
ATOM	7519	C	SER	217	120.976	68.145	28.080	1.00	27.00	B	C
ATOM	7520	O	SER	217	120.694	69.198	28.656	1.00	26.90	B	O
ATOM	7521	N	PRO	218	121.942	67.336	28.523	1.00	26.67	B	N
ATOM	7522	CD	PRO	218	122.469	66.127	27.867	1.00	26.71	B	C
ATOM	7523	CA	PRO	218	122.712	67.646	29.727	1.00	26.69	B	C
ATOM	7524	CB	PRO	218	123.961	66.801	29.547	1.00	27.32	B	C
ATOM	7525	CG	PRO	218	123.385	65.555	28.937	1.00	26.93	B	C
ATOM	7526	C	PRO	218	123.005	69.116	30.010	1.00	27.70	B	C
ATOM	7527	O	PRO	218	122.487	69.661	30.985	1.00	30.37	B	O
ATOM	7528	N	ASN	219	123.818	69.770	29.184	1.00	27.72	B	N
ATOM	7529	CA	ASN	219	124.129	71.176	29.435	1.00	26.82	B	C
ATOM	7530	CB	ASN	219	125.485	71.562	28.816	1.00	26.61	B	C
ATOM	7531	CG	ASN	219	125.447	71.640	27.308	1.00	27.23	B	C
ATOM	7532	OD1	ASN	219	124.376	71.725	26.706	1.00	25.21	B	O
ATOM	7533	ND2	ASN	219	126.626	71.632	26.690	1.00	30.87	B	N
ATOM	7534	C	ASN	219	123.029	72.133	28.958	1.00	27.38	B	C
ATOM	7535	O	ASN	219	123.212	73.351	28.943	1.00	29.12	B	O
ATOM	7536	N	GLY	220	121.888	71.575	28.565	1.00	26.98	B	N
ATOM	7537	CA	GLY	220	120.765	72.391	28.137	1.00	26.30	B	C
ATOM	7538	C	GLY	220	120.823	73.030	26.765	1.00	26.91	B	C
ATOM	7539	O	GLY	220	120.097	73.986	26.500	1.00	27.55	B	O
ATOM	7540	N	THR	221	121.669	72.512	25.884	1.00	27.00	B	N
ATOM	7541	CA	THR	221	121.775	73.073	24.547	1.00	26.99	B	C
ATOM	7542	CB	THR	221	123.052	72.584	23.808	1.00	27.74	B	C
ATOM	7543	OG1	THR	221	124.213	73.084	24.481	1.00	29.49	B	O
ATOM	7544	CG2	THR	221	123.068	73.089	22.367	1.00	26.25	B	C
ATOM	7545	C	THR	221	120.559	72.685	23.730	1.00	26.42	B	C

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## FIG. 4 - 155

(Continued)

ATOM	7546	O	THR	221	119.862	73.551	23.201	1.00	28.29	B	O
ATOM	7547	N	PHE	222	120.305	71.386	23.619	1.00	25.34	B	N
ATOM	7548	CA	PHE	222	119.158	70.921	22.850	1.00	25.13	B	C
ATOM	7549	CB	PHE	222	119.480	69.645	22.069	1.00	25.65	B	C
ATOM	7550	CG	PHE	222	120.722	69.723	21.246	1.00	26.36	B	C
ATOM	7551	CD1	PHE	222	121.955	69.384	21.797	1.00	26.35	B	C
ATOM	7552	CD2	PHE	222	120.661	70.111	19.912	1.00	25.81	B	C
ATOM	7553	CE1	PHE	222	123.115	69.425	21.031	1.00	26.12	B	C
ATOM	7554	CE2	PHE	222	121.815	70.158	19.132	1.00	28.19	B	C
ATOM	7555	CZ	PHE	222	123.046	69.814	19.693	1.00	28.46	B	C
ATOM	7556	C	PHE	222	117.949	70.618	23.723	1.00	24.55	B	C
ATOM	7557	O	PHE	222	118.066	70.282	24.901	1.00	24.38	B	O
ATOM	7558	N	LEU	223	116.780	70.746	23.119	1.00	24.19	B	N
ATOM	7559	CA	LEU	223	115.540	70.442	23.789	1.00	22.85	B	C
ATOM	7560	CB	LEU	223	114.618	71.667	23.878	1.00	21.81	B	C
ATOM	7561	CG	LEU	223	113.248	71.340	24.503	1.00	20.49	B	C
ATOM	7562	CD1	LEU	223	113.469	70.684	25.860	1.00	21.10	B	C
ATOM	7563	CD2	LEU	223	112.389	72.587	24.644	1.00	18.49	B	C
ATOM	7564	C	LEU	223	114.885	69.380	22.934	1.00	23.23	B	C
ATOM	7565	O	LEU	223	114.462	69.650	21.808	1.00	22.62	B	O
ATOM	7566	N	ALA	224	114.834	68.162	23.459	1.00	23.47	B	N
ATOM	7567	CA	ALA	224	114.201	67.062	22.753	1.00	23.08	B	C
ATOM	7568	CB	ALA	224	114.935	65.776	23.038	1.00	24.27	B	C
ATOM	7569	C	ALA	224	112.761	66.968	23.248	1.00	23.38	B	C
ATOM	7570	O	ALA	224	112.498	67.111	24.444	1.00	23.37	B	O
ATOM	7571	N	TYR	225	111.825	66.755	22.328	1.00	23.10	B	N
ATOM	7572	CA	TYR	225	110.423	66.635	22.703	1.00	21.31	B	C
ATOM	7573	CB	TYR	225	109.733	67.997	22.701	1.00	18.23	B	C
ATOM	7574	CG	TYR	225	109.648	68.624	21.332	1.00	18.56	B	C
ATOM	7575	CD1	TYR	225	110.680	69.443	20.849	1.00	16.52	B	C
ATOM	7576	CE1	TYR	225	110.607	70.017	19.589	1.00	13.07	B	C
ATOM	7577	CD2	TYR	225	108.543	68.399	20.509	1.00	16.18	B	C
ATOM	7578	CE2	TYR	225	108.466	68.970	19.244	1.00	14.89	B	C
ATOM	7579	CZ	TYR	225	109.502	69.777	18.796	1.00	12.68	B	C
ATOM	7580	OH	TYR	225	109.431	70.342	17.553	1.00	14.06	B	O
ATOM	7581	C	TYR	225	109.705	65.712	21.737	1.00	21.55	B	C
ATOM	7582	O	TYR	225	110.143	65.523	20.607	1.00	22.86	B	O
ATOM	7583	N	ALA	226	108.596	65.141	22.195	1.00	20.96	B	N
ATOM	7584	CA	ALA	226	107.811	64.235	21.381	1.00	19.66	B	C
ATOM	7585	CB	ALA	226	107.485	62.980	22.173	1.00	19.19	B	C
ATOM	7586	C	ALA	226	106.528	64.921	20.962	1.00	19.73	B	C
ATOM	7587	O	ALA	226	106.107	65.908	21.576	1.00	21.22	B	O
ATOM	7588	N	GLN	227	105.912	64.410	19.909	1.00	16.70	B	N
ATOM	7589	CA	GLN	227	104.659	64.968	19.457	1.00	17.01	B	C
ATOM	7590	CB	GLN	227	104.823	65.709	18.139	1.00	17.47	B	C
ATOM	7591	CG	GLN	227	103.512	66.300	17.670	1.00	18.65	B	C
ATOM	7592	CD	GLN	227	103.554	66.788	16.249	1.00	18.45	B	C
ATOM	7593	OE1	GLN	227	103.724	66.007	15.320	1.00	18.91	B	O
ATOM	7594	NE2	GLN	227	103.394	68.090	16.070	1.00	19.57	B	N

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## FIG. 4 - 156

(Continued)

ATOM	7595	C	GLN	227	103.651	63.841	19.274	1.00	17.21	B	C
ATOM	7596	O	GLN	227	103.931	62.850	18.594	1.00	17.76	B	O
ATOM	7597	N	PHE	228	102.483	63.990	19.888	1.00	16.03	B	N
ATOM	7598	CA	PHE	228	101.447	62.980	19.768	1.00	17.64	B	C
ATOM	7599	CB	PHE	228	100.985	62.524	21.158	1.00	14.78	B	C
ATOM	7600	CG	PHE	228	102.111	62.105	22.065	1.00	13.03	B	C
ATOM	7601	CD1	PHE	228	102.659	63.003	22.982	1.00	12.33	B	C
ATOM	7602	CD2	PHE	228	102.653	60.826	21.978	1.00	12.01	B	C
ATOM	7603	CE1	PHE	228	103.732	62.636	23.796	1.00	9.77	B	C
ATOM	7604	CE2	PHE	228	103.725	60.450	22.786	1.00	11.27	B	C
ATOM	7605	CZ	PHE	228	104.267	61.360	23.698	1.00	9.50	B	C
ATOM	7606	C	PHE	228	100.263	63.523	18.955	1.00	18.96	B	C
ATOM	7607	O	PHE	228	99.894	64.697	19.064	1.00	19.98	B	O
ATOM	7608	N	ASN	229	99.685	62.657	18.133	1.00	20.11	B	N
ATOM	7609	CA	ASN	229	98.548	63.002	17.285	1.00	20.74	B	C
ATOM	7610	CB	ASN	229	98.965	62.867	15.819	1.00	22.98	B	C
ATOM	7611	CG	ASN	229	97.980	63.488	14.867	1.00	27.56	B	C
ATOM	7612	OD1	ASN	229	96.795	63.610	15.174	1.00	31.63	B	O
ATOM	7613	ND2	ASN	229	98.467	63.871	13.692	1.00	30.76	B	N
ATOM	7614	C	ASN	229	97.435	61.995	17.609	1.00	21.10	B	C
ATOM	7615	O	ASN	229	97.550	60.816	17.283	1.00	20.02	B	O
ATOM	7616	N	ASP	230	96.369	62.444	18.260	1.00	22.16	B	N
ATOM	7617	CA	ASP	230	95.277	61.534	18.608	1.00	24.31	B	C
ATOM	7618	CB	ASP	230	94.877	61.683	20.079	1.00	23.86	B	C
ATOM	7619	CG	ASP	230	95.999	61.332	21.027	1.00	25.25	B	C
ATOM	7620	OD1	ASP	230	95.701	60.914	22.159	1.00	27.89	B	O
ATOM	7621	OD2	ASP	230	97.180	61.485	20.656	1.00	27.78	B	O
ATOM	7622	C	ASP	230	94.056	61.776	17.740	1.00	24.83	B	C
ATOM	7623	O	ASP	230	92.927	61.496	18.148	1.00	24.00	B	O
ATOM	7624	N	THR	231	94.297	62.284	16.536	1.00	25.37	B	N
ATOM	7625	CA	THR	231	93.229	62.582	15.593	1.00	26.24	B	C
ATOM	7626	CB	THR	231	93.802	62.868	14.193	1.00	25.71	B	C
ATOM	7627	OG1	THR	231	94.439	64.151	14.194	1.00	26.78	B	O
ATOM	7628	CG2	THR	231	92.702	62.851	13.150	1.00	23.72	B	C
ATOM	7629	C	THR	231	92.148	61.510	15.467	1.00	27.04	B	C
ATOM	7630	O	THR	231	90.964	61.815	15.604	1.00	29.05	B	O
ATOM	7631	N	GLU	232	92.545	60.265	15.211	1.00	27.00	B	N
ATOM	7632	CA	GLU	232	91.574	59.183	15.038	1.00	26.30	B	C
ATOM	7633	CB	GLU	232	92.017	58.286	13.877	1.00	29.71	B	C
ATOM	7634	CG	GLU	232	92.177	59.036	12.563	1.00	36.71	B	C
ATOM	7635	CD	GLU	232	92.971	58.253	11.519	1.00	39.94	B	C
ATOM	7636	OE1	GLU	232	92.434	57.273	10.943	1.00	41.61	B	O
ATOM	7637	OE2	GLU	232	94.142	58.623	11.286	1.00	39.28	B	O
ATOM	7638	C	GLU	232	91.320	58.328	16.282	1.00	23.78	B	C
ATOM	7639	O	GLU	232	90.683	57.280	16.208	1.00	23.18	B	O
ATOM	7640	N	VAL	233	91.823	58.763	17.427	1.00	21.91	B	N
ATOM	7641	CA	VAL	233	91.608	58.010	18.652	1.00	20.18	B	C
ATOM	7642	CB	VAL	233	92.651	58.375	19.727	1.00	20.26	B	C
ATOM	7643	CG1	VAL	233	92.352	57.627	21.016	1.00	18.23	B	C

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(Continued)

## FIG. 4 - 157

ATOM	7644	CG2	VAL	233	94.050	58.032	19.223	1.00	18.80	B	C
ATOM	7645	C	VAL	233	90.218	58.339	19.175	1.00	18.04	B	C
ATOM	7646	O	VAL	233	89.886	59.507	19.378	1.00	19.49	B	O
ATOM	7647	N	PRO	234	89.383	57.315	19.394	1.00	16.04	B	N
ATOM	7648	CD	PRO	234	89.633	55.876	19.231	1.00	14.37	B	C
ATOM	7649	CA	PRO	234	88.025	57.544	19.896	1.00	15.33	B	C
ATOM	7650	CB	PRO	234	87.461	56.133	20.030	1.00	13.91	B	C
ATOM	7651	CG	PRO	234	88.247	55.363	19.013	1.00	12.89	B	C
ATOM	7652	C	PRO	234	88.048	58.275	21.227	1.00	14.45	B	C
ATOM	7653	O	PRO	234	89.043	58.242	21.950	1.00	13.13	B	O
ATOM	7654	N	LEU	235	86.941	58.927	21.547	1.00	14.92	B	N
ATOM	7655	CA	LEU	235	86.831	59.676	22.791	1.00	13.91	B	C
ATOM	7656	CB	LEU	235	86.131	61.005	22.536	1.00	14.93	B	C
ATOM	7657	CG	LEU	235	86.627	61.937	21.434	1.00	16.83	B	C
ATOM	7658	CD1	LEU	235	85.581	63.030	21.198	1.00	17.90	B	C
ATOM	7659	CD2	LEU	235	87.963	62.534	21.833	1.00	14.85	B	C
ATOM	7660	C	LEU	235	85.998	58.911	23.803	1.00	12.70	B	C
ATOM	7661	O	LEU	235	84.941	58.385	23.456	1.00	13.27	B	O
ATOM	7662	N	ILE	236	86.468	58.801	25.039	1.00	10.71	B	N
ATOM	7663	CA	ILE	236	85.618	58.165	26.037	1.00	10.96	B	C
ATOM	7664	CB	ILE	236	86.385	57.630	27.283	1.00	9.70	B	C
ATOM	7665	CG2	ILE	236	87.316	58.692	27.859	1.00	10.05	B	C
ATOM	7666	CG1	ILE	236	85.386	57.246	28.371	1.00	7.51	B	C
ATOM	7667	CD1	ILE	236	84.465	56.100	28.002	1.00	9.77	B	C
ATOM	7668	C	ILE	236	84.774	59.369	26.456	1.00	12.91	B	C
ATOM	7669	O	ILE	236	85.277	60.500	26.486	1.00	13.64	B	O
ATOM	7670	N	GLU	237	83.497	59.156	26.741	1.00	13.69	B	N
ATOM	7671	CA	GLU	237	82.651	60.267	27.150	1.00	14.30	B	C
ATOM	7672	CB	GLU	237	81.657	60.643	26.041	1.00	15.93	B	C
ATOM	7673	CG	GLU	237	82.307	60.993	24.708	1.00	20.06	B	C
ATOM	7674	CD	GLU	237	81.311	61.541	23.682	1.00	24.67	B	C
ATOM	7675	OE1	GLU	237	80.133	61.125	23.713	1.00	27.11	B	O
ATOM	7676	OE2	GLU	237	81.706	62.377	22.832	1.00	25.71	B	O
ATOM	7677	C	GLU	237	81.902	59.898	28.407	1.00	12.26	B	C
ATOM	7678	O	GLU	237	81.473	58.759	28.569	1.00	12.02	B	O
ATOM	7679	N	TYR	238	81.768	60.860	29.310	1.00	12.67	B	N
ATOM	7680	CA	TYR	238	81.044	60.630	30.550	1.00	13.08	B	C
ATOM	7681	CB	TYR	238	81.903	59.816	31.534	1.00	11.88	B	C
ATOM	7682	CG	TYR	238	83.201	60.458	31.954	1.00	15.20	B	C
ATOM	7683	CD1	TYR	238	83.250	61.347	33.026	1.00	15.46	B	C
ATOM	7684	CE1	TYR	238	84.458	61.920	33.430	1.00	15.78	B	C
ATOM	7685	CD2	TYR	238	84.390	60.160	31.291	1.00	14.07	B	C
ATOM	7686	CE2	TYR	238	85.592	60.727	31.683	1.00	14.24	B	C
ATOM	7687	CZ	TYR	238	85.623	61.606	32.751	1.00	13.94	B	C
ATOM	7688	OH	TYR	238	86.818	62.173	33.129	1.00	12.45	B	O
ATOM	7689	C	TYR	238	80.583	61.944	31.163	1.00	13.53	B	C
ATOM	7690	O	TYR	238	81.095	63.008	30.832	1.00	14.88	B	O
ATOM	7691	N	SER	239	79.592	61.865	32.042	1.00	14.64	B	N
ATOM	7692	CA	SER	239	79.040	63.047	32.684	1.00	13.89	B	C

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## FIG. 4 - 158

(Continued)

ATOM	7693	CB	SER	239	77.597	62.783	33.085	1.00	13.29	B	C
ATOM	7694	OG	SER	239	76.800	62.496	31.961	1.00	19.37	B	O
ATOM	7695	C	SER	239	79.775	63.547	33.915	1.00	14.65	B	C
ATOM	7696	O	SER	239	80.361	62.775	34.673	1.00	15.52	B	O
ATOM	7697	N	PHE	240	79.737	64.860	34.100	1.00	14.89	B	N
ATOM	7698	CA	PHE	240	80.313	65.493	35.276	1.00	15.60	B	C
ATOM	7699	CB	PHE	240	81.543	66.325	34.932	1.00	17.00	B	C
ATOM	7700	CG	PHE	240	82.422	66.591	36.112	1.00	14.96	B	C
ATOM	7701	CD1	PHE	240	83.325	65.629	36.547	1.00	15.66	B	C
ATOM	7702	CD2	PHE	240	82.312	67.781	36.822	1.00	14.41	B	C
ATOM	7703	CE1	PHE	240	84.108	65.846	37.675	1.00	13.32	B	C
ATOM	7704	CE2	PHE	240	83.087	68.009	37.950	1.00	12.45	B	C
ATOM	7705	CZ	PHE	240	83.988	67.039	38.379	1.00	11.23	B	C
ATOM	7706	C	PHE	240	79.184	66.403	35.758	1.00	15.75	B	C
ATOM	7707	O	PHE	240	78.671	67.232	34.995	1.00	14.05	B	O
ATOM	7708	N	TYR	241	78.785	66.231	37.013	1.00	15.13	B	N
ATOM	7709	CA	TYR	241	77.683	67.002	37.567	1.00	14.92	B	C
ATOM	7710	CB	TYR	241	76.912	66.125	38.545	1.00	13.15	B	C
ATOM	7711	CG	TYR	241	76.480	64.848	37.880	1.00	12.77	B	C
ATOM	7712	CD1	TYR	241	75.393	64.832	37.007	1.00	11.36	B	C
ATOM	7713	CE1	TYR	241	75.051	63.678	36.304	1.00	12.47	B	C
ATOM	7714	CD2	TYR	241	77.215	63.674	38.041	1.00	12.85	B	C
ATOM	7715	CE2	TYR	241	76.883	62.512	37.342	1.00	12.55	B	C
ATOM	7716	CZ	TYR	241	75.801	62.523	36.472	1.00	12.41	B	C
ATOM	7717	OH	TYR	241	75.489	61.395	35.748	1.00	12.90	B	O
ATOM	7718	C	TYR	241	78.100	68.299	38.208	1.00	15.24	B	C
ATOM	7719	O	TYR	241	77.311	69.239	38.263	1.00	17.04	B	O
ATOM	7720	N	SER	242	79.337	68.353	38.694	1.00	16.92	B	N
ATOM	7721	CA	SER	242	79.864	69.570	39.305	1.00	16.89	B	C
ATOM	7722	CB	SER	242	79.816	70.707	38.280	1.00	15.48	B	C
ATOM	7723	OG	SER	242	80.439	71.870	38.782	1.00	18.12	B	O
ATOM	7724	C	SER	242	79.078	69.963	40.548	1.00	16.70	B	C
ATOM	7725	O	SER	242	78.438	69.121	41.171	1.00	18.07	B	O
ATOM	7726	N	ASP	243	79.136	71.241	40.912	1.00	17.57	B	N
ATOM	7727	CA	ASP	243	78.405	71.728	42.075	1.00	19.72	B	C
ATOM	7728	CB	ASP	243	78.846	73.142	42.442	1.00	23.43	B	C
ATOM	7729	CG	ASP	243	80.275	73.188	42.950	1.00	28.70	B	C
ATOM	7730	OD1	ASP	243	80.646	72.307	43.765	1.00	29.62	B	O
ATOM	7731	OD2	ASP	243	81.021	74.106	42.542	1.00	29.69	B	O
ATOM	7732	C	ASP	243	76.917	71.708	41.772	1.00	20.24	B	C
ATOM	7733	O	ASP	243	76.508	71.777	40.609	1.00	20.38	B	O
ATOM	7734	N	GLU	244	76.104	71.624	42.818	1.00	19.25	B	N
ATOM	7735	CA	GLU	244	74.668	71.545	42.630	1.00	19.29	B	C
ATOM	7736	CB	GLU	244	73.966	71.376	43.988	1.00	19.46	B	C
ATOM	7737	CG	GLU	244	73.283	72.609	44.533	1.00	23.65	B	C
ATOM	7738	CD	GLU	244	72.567	72.334	45.847	1.00	26.30	B	C
ATOM	7739	OE1	GLU	244	73.225	71.856	46.797	1.00	28.64	B	O
ATOM	7740	OE2	GLU	244	71.349	72.595	45.934	1.00	27.72	B	O
ATOM	7741	C	GLU	244	74.086	72.720	41.850	1.00	18.30	B	C

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## FIG. 4 - 159

(Continued)

ATOM	7742	O	GLU	244	72.958	72.647	41.355	1.00	19.81	B	O
ATOM	7743	N	SER	245	74.861	73.785	41.702	1.00	15.52	B	N
ATOM	7744	CA	SER	245	74.381	74.958	40.986	1.00	11.95	B	C
ATOM	7745	CB	SER	245	75.157	76.196	41.425	1.00	11.90	B	C
ATOM	7746	OG	SER	245	76.473	76.162	40.915	1.00	17.74	B	O
ATOM	7747	C	SER	245	74.459	74.821	39.470	1.00	9.32	B	C
ATOM	7748	O	SER	245	73.883	75.625	38.752	1.00	10.56	B	O
ATOM	7749	N	LEU	246	75.167	73.819	38.968	1.00	8.50	B	N
ATOM	7750	CA	LEU	246	75.252	73.647	37.518	1.00	8.56	B	C
ATOM	7751	CB	LEU	246	76.481	72.812	37.145	1.00	8.57	B	C
ATOM	7752	CG	LEU	246	76.770	72.639	35.644	1.00	11.81	B	C
ATOM	7753	CD1	LEU	246	77.074	73.984	35.008	1.00	5.99	B	C
ATOM	7754	CD2	LEU	246	77.949	71.694	35.449	1.00	10.70	B	C
ATOM	7755	C	LEU	246	73.971	72.944	37.070	1.00	10.18	B	C
ATOM	7756	O	LEU	246	73.772	71.758	37.349	1.00	9.30	B	O
ATOM	7757	N	GLN	247	73.094	73.685	36.393	1.00	12.01	B	N
ATOM	7758	CA	GLN	247	71.815	73.144	35.938	1.00	12.00	B	C
ATOM	7759	CB	GLN	247	70.995	74.230	35.245	1.00	12.36	B	C
ATOM	7760	CG	GLN	247	69.584	73.806	34.884	1.00	14.88	B	C
ATOM	7761	CD	GLN	247	68.727	74.978	34.446	1.00	16.57	B	C
ATOM	7762	OE1	GLN	247	69.152	75.790	33.627	1.00	18.02	B	O
ATOM	7763	NE2	GLN	247	67.512	75.069	34.986	1.00	13.91	B	N
ATOM	7764	C	GLN	247	71.974	71.942	35.022	1.00	12.63	B	C
ATOM	7765	O	GLN	247	71.358	70.903	35.249	1.00	13.50	B	O
ATOM	7766	N	TYR	248	72.793	72.074	33.987	1.00	13.12	B	N
ATOM	7767	CA	TYR	248	73.022	70.949	33.089	1.00	13.90	B	C
ATOM	7768	CB	TYR	248	72.954	71.379	31.628	1.00	11.81	B	C
ATOM	7769	CG	TYR	248	71.562	71.727	31.155	1.00	11.76	B	C
ATOM	7770	CD1	TYR	248	70.967	72.942	31.498	1.00	10.54	B	C
ATOM	7771	CE1	TYR	248	69.689	73.265	31.055	1.00	11.01	B	C
ATOM	7772	CD2	TYR	248	70.842	70.843	30.360	1.00	9.97	B	C
ATOM	7773	CE2	TYR	248	69.562	71.155	29.911	1.00	11.67	B	C
ATOM	7774	CZ	TYR	248	68.989	72.366	30.259	1.00	11.89	B	C
ATOM	7775	OH	TYR	248	67.722	72.674	29.801	1.00	10.14	B	O
ATOM	7776	C	TYR	248	74.385	70.340	33.353	1.00	14.77	B	C
ATOM	7777	O	TYR	248	75.384	71.049	33.419	1.00	15.30	B	O
ATOM	7778	N	PRO	249	74.441	69.014	33.544	1.00	15.88	B	N
ATOM	7779	CD	PRO	249	73.350	68.031	33.636	1.00	15.23	B	C
ATOM	7780	CA	PRO	249	75.739	68.381	33.793	1.00	16.47	B	C
ATOM	7781	CB	PRO	249	75.360	66.947	34.161	1.00	16.57	B	C
ATOM	7782	CG	PRO	249	74.086	66.732	33.417	1.00	15.37	B	C
ATOM	7783	C	PRO	249	76.568	68.468	32.515	1.00	16.66	B	C
ATOM	7784	O	PRO	249	76.016	68.446	31.419	1.00	15.91	B	O
ATOM	7785	N	LYS	250	77.884	68.586	32.647	1.00	16.70	B	N
ATOM	7786	CA	LYS	250	78.721	68.683	31.463	1.00	18.05	B	C
ATOM	7787	CB	LYS	250	79.920	69.591	31.719	1.00	17.36	B	C
ATOM	7788	CG	LYS	250	80.912	69.015	32.681	1.00	22.33	B	C
ATOM	7789	CD	LYS	250	82.204	69.826	32.691	1.00	28.25	B	C
ATOM	7790	CE	LYS	250	82.952	69.757	31.355	1.00	26.52	B	C

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(Continued)

## FIG. 4 - 160

ATOM	7791	NZ	LYS	250	84.262	70.465	31.442	1.00	26.19	B	N
ATOM	7792	C	LYS	250	79.215	67.313	31.040	1.00	17.64	B	C
ATOM	7793	O	LYS	250	79.348	66.409	31.867	1.00	20.20	B	O
ATOM	7794	N	THR	251	79.478	67.160	29.750	1.00	15.06	B	N
ATOM	7795	CA	THR	251	79.978	65.905	29.234	1.00	14.91	B	C
ATOM	7796	CB	THR	251	79.317	65.537	27.896	1.00	13.86	B	C
ATOM	7797	OG1	THR	251	77.965	65.144	28.128	1.00	14.97	B	O
ATOM	7798	CG2	THR	251	80.058	64.389	27.227	1.00	13.23	B	C
ATOM	7799	C	THR	251	81.473	66.016	29.015	1.00	15.66	B	C
ATOM	7800	O	THR	251	81.934	66.831	28.227	1.00	18.88	B	O
ATOM	7801	N	VAL	252	82.231	65.194	29.720	1.00	15.28	B	N
ATOM	7802	CA	VAL	252	83.675	65.195	29.578	1.00	15.13	B	C
ATOM	7803	CB	VAL	252	84.335	64.717	30.882	1.00	13.64	B	C
ATOM	7804	CG1	VAL	252	85.827	64.580	30.706	1.00	10.22	B	C
ATOM	7805	CG2	VAL	252	84.012	65.701	31.991	1.00	11.83	B	C
ATOM	7806	C	VAL	252	84.027	64.264	28.422	1.00	17.21	B	C
ATOM	7807	O	VAL	252	83.472	63.173	28.304	1.00	17.34	B	O
ATOM	7808	N	ARG	253	84.929	64.710	27.557	1.00	18.91	B	N
ATOM	7809	CA	ARG	253	85.349	63.922	26.403	1.00	20.46	B	C
ATOM	7810	CB	ARG	253	84.822	64.560	25.113	1.00	22.21	B	C
ATOM	7811	CG	ARG	253	83.399	64.137	24.755	1.00	26.72	B	C
ATOM	7812	CD	ARG	253	82.847	64.920	23.578	1.00	28.87	B	C
ATOM	7813	NE	ARG	253	82.176	66.132	24.033	1.00	36.20	B	N
ATOM	7814	CZ	ARG	253	80.870	66.221	24.278	1.00	38.47	B	C
ATOM	7815	NH1	ARG	253	80.084	65.164	24.099	1.00	39.84	B	N
ATOM	7816	NH2	ARG	253	80.352	67.360	24.727	1.00	37.97	B	N
ATOM	7817	C	ARG	253	86.863	63.863	26.389	1.00	19.71	B	C
ATOM	7818	O	ARG	253	87.520	64.886	26.246	1.00	21.87	B	O
ATOM	7819	N	VAL	254	87.404	62.656	26.538	1.00	18.34	B	N
ATOM	7820	CA	VAL	254	88.847	62.434	26.594	1.00	15.15	B	C
ATOM	7821	CB	VAL	254	89.257	61.924	27.994	1.00	16.16	B	C
ATOM	7822	CG1	VAL	254	90.771	61.759	28.081	1.00	15.18	B	C
ATOM	7823	CG2	VAL	254	88.736	62.868	29.065	1.00	16.46	B	C
ATOM	7824	C	VAL	254	89.313	61.397	25.585	1.00	14.67	B	C
ATOM	7825	O	VAL	254	88.806	60.272	25.566	1.00	14.87	B	O
ATOM	7826	N	PRO	255	90.281	61.757	24.726	1.00	13.62	B	N
ATOM	7827	CD	PRO	255	90.872	63.081	24.472	1.00	12.90	B	C
ATOM	7828	CA	PRO	255	90.760	60.777	23.746	1.00	12.62	B	C
ATOM	7829	CB	PRO	255	91.786	61.566	22.933	1.00	11.40	B	C
ATOM	7830	CG	PRO	255	91.263	62.969	23.013	1.00	11.65	B	C
ATOM	7831	C	PRO	255	91.379	59.645	24.553	1.00	12.46	B	C
ATOM	7832	O	PRO	255	92.355	59.831	25.282	1.00	13.25	B	O
ATOM	7833	N	TYR	256	90.796	58.469	24.414	1.00	12.53	B	N
ATOM	7834	CA	TYR	256	91.217	57.306	25.161	1.00	12.05	B	C
ATOM	7835	CB	TYR	256	90.319	57.205	26.398	1.00	12.42	B	C
ATOM	7836	CG	TYR	256	90.608	56.082	27.360	1.00	14.53	B	C
ATOM	7837	CD1	TYR	256	91.021	56.355	28.662	1.00	16.44	B	C
ATOM	7838	CE1	TYR	256	91.192	55.337	29.596	1.00	17.38	B	C
ATOM	7839	CD2	TYR	256	90.382	54.752	27.010	1.00	15.31	B	C

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## FIG. 4 - 161

(Continued)

ATOM	7840	CE2	TYR	256	90.548	53.724	27.941	1.00	16.91	B	C
ATOM	7841	CZ	TYR	256	90.949	54.030	29.232	1.00	16.54	B	C
ATOM	7842	OH	TYR	256	91.068	53.042	30.176	1.00	17.03	B	O
ATOM	7843	C	TYR	256	91.040	56.094	24.263	1.00	11.63	B	C
ATOM	7844	O	TYR	256	89.923	55.765	23.870	1.00	13.76	B	O
ATOM	7845	N	PRO	257	92.141	55.415	23.924	1.00	10.78	B	N
ATOM	7846	CD	PRO	257	93.535	55.786	24.231	1.00	9.21	B	C
ATOM	7847	CA	PRO	257	92.098	54.229	23.068	1.00	9.97	B	C
ATOM	7848	CB	PRO	257	93.473	54.233	22.438	1.00	8.95	B	C
ATOM	7849	CG	PRO	257	94.326	54.657	23.606	1.00	8.91	B	C
ATOM	7850	C	PRO	257	91.859	52.949	23.869	1.00	11.12	B	C
ATOM	7851	O	PRO	257	92.694	52.556	24.681	1.00	9.90	B	O
ATOM	7852	N	LYS	258	90.723	52.300	23.648	1.00	11.97	B	N
ATOM	7853	CA	LYS	258	90.444	51.057	24.353	1.00	13.52	B	C
ATOM	7854	CB	LYS	258	88.930	50.855	24.492	1.00	15.66	B	C
ATOM	7855	CG	LYS	258	88.305	51.808	25.522	1.00	14.41	B	C
ATOM	7856	CD	LYS	258	86.801	51.730	25.552	1.00	18.08	B	C
ATOM	7857	CE	LYS	258	86.204	52.655	26.627	1.00	19.12	B	C
ATOM	7858	NZ	LYS	258	86.355	52.156	28.030	1.00	14.62	B	N
ATOM	7859	C	LYS	258	91.101	49.934	23.571	1.00	14.64	B	C
ATOM	7860	O	LYS	258	91.522	50.139	22.437	1.00	16.07	B	O
ATOM	7861	N	ALA	259	91.227	48.760	24.178	1.00	16.22	B	N
ATOM	7862	CA	ALA	259	91.874	47.627	23.515	1.00	14.83	B	C
ATOM	7863	CB	ALA	259	91.564	46.356	24.261	1.00	14.32	B	C
ATOM	7864	C	ALA	259	91.476	47.476	22.045	1.00	16.09	B	C
ATOM	7865	O	ALA	259	90.293	47.415	21.710	1.00	15.64	B	O
ATOM	7866	N	GLY	260	92.477	47.428	21.172	1.00	15.95	B	N
ATOM	7867	CA	GLY	260	92.221	47.269	19.754	1.00	15.99	B	C
ATOM	7868	C	GLY	260	91.841	48.523	18.982	1.00	17.08	B	C
ATOM	7869	O	GLY	260	91.781	48.488	17.752	1.00	18.87	B	O
ATOM	7870	N	ALA	261	91.587	49.629	19.673	1.00	14.62	B	N
ATOM	7871	CA	ALA	261	91.198	50.851	18.983	1.00	14.89	B	C
ATOM	7872	CB	ALA	261	90.557	51.830	19.963	1.00	13.58	B	C
ATOM	7873	C	ALA	261	92.379	51.509	18.292	1.00	17.12	B	C
ATOM	7874	O	ALA	261	93.489	50.986	18.298	1.00	20.05	B	O
ATOM	7875	N	VAL	262	92.135	52.662	17.686	1.00	17.34	B	N
ATOM	7876	CA	VAL	262	93.192	53.384	17.004	1.00	16.00	B	C
ATOM	7877	CB	VAL	262	92.614	54.371	15.947	1.00	14.51	B	C
ATOM	7878	CG1	VAL	262	93.717	55.252	15.383	1.00	13.59	B	C
ATOM	7879	CG2	VAL	262	91.970	53.596	14.820	1.00	10.82	B	C
ATOM	7880	C	VAL	262	93.984	54.150	18.055	1.00	17.31	B	C
ATOM	7881	O	VAL	262	93.432	54.973	18.786	1.00	20.51	B	O
ATOM	7882	N	ASN	263	95.275	53.856	18.128	1.00	16.87	B	N
ATOM	7883	CA	ASN	263	96.190	54.493	19.068	1.00	17.45	B	C
ATOM	7884	CB	ASN	263	97.406	53.595	19.292	1.00	17.58	B	C
ATOM	7885	CG	ASN	263	97.230	52.629	20.437	1.00	20.08	B	C
ATOM	7886	OD1	ASN	263	97.919	51.606	20.500	1.00	19.88	B	O
ATOM	7887	ND2	ASN	263	96.329	52.950	21.365	1.00	18.44	B	N
ATOM	7888	C	ASN	263	96.706	55.827	18.533	1.00	18.01	B	C

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(Continued)

ATOM	7889	O	ASN	263	96.578	56.134	17.345	1.00	19.39	B	O
ATOM	7890	N	PRO	264	97.288	56.646	19.413	1.00	17.06	B	N
ATOM	7891	CD	PRO	264	97.357	56.546	20.883	1.00	15.68	B	C
ATOM	7892	CA	PRO	264	97.819	57.926	18.950	1.00	15.10	B	C
ATOM	7893	CB	PRO	264	98.089	58.676	20.251	1.00	14.78	B	C
ATOM	7894	CG	PRO	264	98.411	57.569	21.214	1.00	14.94	B	C
ATOM	7895	C	PRO	264	99.105	57.605	18.198	1.00	15.50	B	C
ATOM	7896	O	PRO	264	99.669	56.527	18.369	1.00	15.27	B	O
ATOM	7897	N	THR	265	99.560	58.521	17.354	1.00	16.21	B	N
ATOM	7898	CA	THR	265	100.796	58.305	16.617	1.00	15.30	B	C
ATOM	7899	CB	THR	265	100.647	58.677	15.132	1.00	15.20	B	C
ATOM	7900	OG1	THR	265	100.081	59.983	15.029	1.00	17.05	B	O
ATOM	7901	CG2	THR	265	99.747	57.687	14.415	1.00	10.60	B	C
ATOM	7902	C	THR	265	101.818	59.211	17.279	1.00	16.13	B	C
ATOM	7903	O	THR	265	101.454	60.126	18.007	1.00	16.83	B	O
ATOM	7904	N	VAL	266	103.095	58.971	17.030	1.00	17.64	B	N
ATOM	7905	CA	VAL	266	104.118	59.781	17.667	1.00	17.49	B	C
ATOM	7906	CB	VAL	266	104.626	59.060	18.930	1.00	15.28	B	C
ATOM	7907	CG1	VAL	266	105.224	57.714	18.538	1.00	12.10	B	C
ATOM	7908	CG2	VAL	266	105.642	59.921	19.666	1.00	12.62	B	C
ATOM	7909	C	VAL	266	105.312	60.112	16.769	1.00	19.23	B	C
ATOM	7910	O	VAL	266	105.693	59.331	15.893	1.00	18.24	B	O
ATOM	7911	N	LYS	267	105.889	61.287	17.003	1.00	20.19	B	N
ATOM	7912	CA	LYS	267	107.058	61.756	16.272	1.00	19.42	B	C
ATOM	7913	CB	LYS	267	106.678	62.855	15.291	1.00	19.76	B	C
ATOM	7914	CG	LYS	267	105.786	62.413	14.168	1.00	21.59	B	C
ATOM	7915	CD	LYS	267	105.452	63.605	13.291	1.00	23.15	B	C
ATOM	7916	CE	LYS	267	104.593	63.205	12.119	1.00	23.47	B	C
ATOM	7917	NZ	LYS	267	104.225	64.402	11.334	1.00	27.20	B	N
ATOM	7918	C	LYS	267	108.032	62.334	17.288	1.00	19.59	B	C
ATOM	7919	O	LYS	267	107.618	62.826	18.336	1.00	20.86	B	O
ATOM	7920	N	PHE	268	109.322	62.275	16.984	1.00	19.32	B	N
ATOM	7921	CA	PHE	268	110.325	62.818	17.882	1.00	18.94	B	C
ATOM	7922	CB	PHE	268	111.350	61.757	18.259	1.00	17.47	B	C
ATOM	7923	CG	PHE	268	112.186	62.131	19.444	1.00	16.21	B	C
ATOM	7924	CD1	PHE	268	111.601	62.290	20.692	1.00	16.98	B	C
ATOM	7925	CD2	PHE	268	113.555	62.327	19.313	1.00	16.35	B	C
ATOM	7926	CE1	PHE	268	112.368	62.639	21.797	1.00	18.80	B	C
ATOM	7927	CE2	PHE	268	114.332	62.674	20.405	1.00	17.68	B	C
ATOM	7928	CZ	PHE	268	113.737	62.832	21.655	1.00	18.66	B	C
ATOM	7929	C	PHE	268	111.016	63.979	17.192	1.00	20.34	B	C
ATOM	7930	O	PHE	268	111.114	64.016	15.968	1.00	21.73	B	O
ATOM	7931	N	PHE	269	111.491	64.931	17.981	1.00	20.76	B	N
ATOM	7932	CA	PHE	269	112.152	66.105	17.435	1.00	20.74	B	C
ATOM	7933	CB	PHE	269	111.141	67.239	17.222	1.00	19.80	B	C
ATOM	7934	CG	PHE	269	110.070	66.937	16.216	1.00	21.88	B	C
ATOM	7935	CD1	PHE	269	110.332	67.019	14.853	1.00	22.75	B	C
ATOM	7936	CD2	PHE	269	108.785	66.605	16.631	1.00	23.20	B	C
ATOM	7937	CE1	PHE	269	109.326	66.781	13.912	1.00	21.98	B	C

(Continued)

## FIG. 4 - 163

ATOM	7938	CE2	PHE	269	107.771	66.364	15.700	1.00	23.06	B	C
ATOM	7939	CZ	PHE	269	108.044	66.454	14.337	1.00	22.44	B	C
ATOM	7940	C	PHE	269	113.209	66.606	18.402	1.00	21.66	B	C
ATOM	7941	O	PHE	269	113.127	66.376	19.613	1.00	21.27	B	O
ATOM	7942	N	VAL	270	114.195	67.305	17.858	1.00	21.99	B	N
ATOM	7943	CA	VAL	270	115.239	67.896	18.667	1.00	23.26	B	C
ATOM	7944	CB	VAL	270	116.527	67.062	18.635	1.00	23.10	B	C
ATOM	7945	CG1	VAL	270	117.517	67.624	19.630	1.00	23.57	B	C
ATOM	7946	CG2	VAL	270	116.219	65.609	18.985	1.00	23.02	B	C
ATOM	7947	C	VAL	270	115.495	69.285	18.095	1.00	25.32	B	C
ATOM	7948	O	VAL	270	115.600	69.460	16.880	1.00	26.00	B	O
ATOM	7949	N	VAL	271	115.561	70.278	18.973	1.00	26.96	B	N
ATOM	7950	CA	VAL	271	115.794	71.650	18.546	1.00	27.45	B	C
ATOM	7951	CB	VAL	271	114.516	72.514	18.714	1.00	28.95	B	C
ATOM	7952	CG1	VAL	271	114.096	72.563	20.177	1.00	28.40	B	C
ATOM	7953	CG2	VAL	271	114.769	73.915	18.186	1.00	29.54	B	C
ATOM	7954	C	VAL	271	116.926	72.258	19.363	1.00	27.39	B	C
ATOM	7955	O	VAL	271	117.094	71.935	20.536	1.00	26.71	B	O
ATOM	7956	N	ASN	272	117.706	73.128	18.728	1.00	27.87	B	N
ATOM	7957	CA	ASN	272	118.828	73.788	19.383	1.00	27.39	B	C
ATOM	7958	CB	ASN	272	119.951	74.056	18.378	1.00	27.64	B	C
ATOM	7959	CG	ASN	272	121.179	74.672	19.031	1.00	29.11	B	C
ATOM	7960	OD1	ASN	272	121.094	75.706	19.696	1.00	28.35	B	O
ATOM	7961	ND2	ASN	272	122.330	74.036	18.841	1.00	30.38	B	N
ATOM	7962	C	ASN	272	118.347	75.104	19.972	1.00	27.43	B	C
ATOM	7963	O	ASN	272	117.943	76.012	19.243	1.00	27.41	B	O
ATOM	7964	N	THR	273	118.397	75.208	21.292	1.00	27.62	B	N
ATOM	7965	CA	THR	273	117.938	76.411	21.959	1.00	28.77	B	C
ATOM	7966	CB	THR	273	117.509	76.100	23.400	1.00	27.46	B	C
ATOM	7967	OG1	THR	273	118.653	75.727	24.181	1.00	28.06	B	O
ATOM	7968	CG2	THR	273	116.510	74.960	23.403	1.00	26.33	B	C
ATOM	7969	C	THR	273	118.988	77.516	21.967	1.00	31.23	B	C
ATOM	7970	O	THR	273	118.669	78.680	22.208	1.00	32.66	B	O
ATOM	7971	N	ASP	274	120.239	77.157	21.698	1.00	32.45	B	N
ATOM	7972	CA	ASP	274	121.315	78.139	21.676	1.00	33.79	B	C
ATOM	7973	CB	ASP	274	122.671	77.446	21.775	1.00	34.63	B	C
ATOM	7974	CG	ASP	274	123.019	77.049	23.193	1.00	36.82	B	C
ATOM	7975	OD1	ASP	274	124.047	76.363	23.385	1.00	37.48	B	O
ATOM	7976	OD2	ASP	274	122.267	77.430	24.117	1.00	37.18	B	O
ATOM	7977	C	ASP	274	121.277	78.996	20.419	1.00	35.09	B	C
ATOM	7978	O	ASP	274	121.899	80.058	20.366	1.00	34.53	B	O
ATOM	7979	N	SER	275	120.540	78.542	19.412	1.00	35.53	B	N
ATOM	7980	CA	SER	275	120.456	79.279	18.166	1.00	37.39	B	C
ATOM	7981	CB	SER	275	121.096	78.462	17.051	1.00	36.90	B	C
ATOM	7982	OG	SER	275	120.476	77.197	16.948	1.00	41.05	B	O
ATOM	7983	C	SER	275	119.030	79.652	17.781	1.00	39.58	B	C
ATOM	7984	O	SER	275	118.580	79.355	16.673	1.00	40.66	B	O
ATOM	7985	N	LEU	276	118.323	80.311	18.695	1.00	40.56	B	N
ATOM	7986	CA	LEU	276	116.949	80.732	18.443	1.00	40.53	B	C

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## FIG. 4 - 164

(Continued)

ATOM	7987	CB	LEU	276	116.076	80.425	19.664	1.00	38.58	B	C
ATOM	7988	CG	LEU	276	116.002	78.958	20.097	1.00	36.34	B	C
ATOM	7989	CD1	LEU	276	115.319	78.876	21.445	1.00	35.16	B	C
ATOM	7990	CD2	LEU	276	115.261	78.134	19.057	1.00	32.57	B	C
ATOM	7991	C	LEU	276	116.914	82.229	18.140	1.00	41.99	B	C
ATOM	7992	O	LEU	276	117.675	83.002	18.721	1.00	41.16	B	C
ATOM	7993	N	SER	277	116.029	82.634	17.233	1.00	44.02	B	O
ATOM	7994	CA	SER	277	115.916	84.044	16.863	1.00	46.53	B	N
ATOM	7995	CB	SER	277	116.489	84.277	15.462	1.00	48.49	B	C
ATOM	7996	OG	SER	277	116.268	85.618	15.044	1.00	50.90	B	C
ATOM	7997	C	SER	277	114.494	84.586	16.902	1.00	46.23	B	O
ATOM	7998	O	SER	277	113.529	83.856	16.701	1.00	46.82	B	C
ATOM	7999	N	SER	278	114.378	85.884	17.148	1.00	46.94	B	O
ATOM	8000	CA	SER	278	113.081	86.535	17.202	1.00	47.82	B	N
ATOM	8001	CB	SER	278	113.204	87.899	17.884	1.00	48.09	B	C
ATOM	8002	OG	SER	278	113.617	87.759	19.234	1.00	49.14	B	C
ATOM	8003	C	SER	278	112.531	86.710	15.794	1.00	48.26	B	O
ATOM	8004	O	SER	278	111.325	86.829	15.600	1.00	48.73	B	C
ATOM	8005	N	VAL	279	113.419	86.723	14.808	1.00	48.48	B	O
ATOM	8006	CA	VAL	279	112.995	86.889	13.428	1.00	48.89	B	N
ATOM	8007	CB	VAL	279	114.189	87.229	12.514	1.00	49.95	B	C
ATOM	8008	CG1	VAL	279	113.709	87.454	11.089	1.00	50.61	B	C
ATOM	8009	CG2	VAL	279	114.902	88.464	13.037	1.00	50.28	B	C
ATOM	8010	C	VAL	279	112.340	85.606	12.941	1.00	48.52	B	C
ATOM	8011	O	VAL	279	111.130	85.433	13.082	1.00	49.49	B	O
ATOM	8012	N	THR	280	113.145	84.708	12.380	1.00	47.70	B	N
ATOM	8013	CA	THR	280	112.651	83.432	11.872	1.00	46.64	B	C
ATOM	8014	CB	THR	280	113.719	82.709	11.032	1.00	47.86	B	C
ATOM	8015	OG1	THR	280	113.179	81.479	10.531	1.00	48.07	B	O
ATOM	8016	CG2	THR	280	114.946	82.399	11.883	1.00	47.49	B	C
ATOM	8017	C	THR	280	112.238	82.484	12.992	1.00	45.40	B	C
ATOM	8018	O	THR	280	112.586	82.677	14.155	1.00	44.24	B	O
ATOM	8019	N	ASN	281	111.499	81.447	12.622	1.00	45.09	B	N
ATOM	8020	CA	ASN	281	111.040	80.454	13.581	1.00	44.81	B	C
ATOM	8021	CB	ASN	281	109.744	79.815	13.089	1.00	46.08	B	C
ATOM	8022	CG	ASN	281	108.592	80.786	13.096	1.00	48.90	B	C
ATOM	8023	OD1	ASN	281	108.351	81.455	14.101	1.00	49.62	B	O
ATOM	8024	ND2	ASN	281	107.873	80.868	11.984	1.00	52.14	B	N
ATOM	8025	C	ASN	281	112.088	79.379	13.812	1.00	43.47	B	C
ATOM	8026	O	ASN	281	112.874	79.065	12.919	1.00	44.44	B	O
ATOM	8027	N	ALA	282	112.100	78.823	15.019	1.00	41.76	B	N
ATOM	8028	CA	ALA	282	113.045	77.773	15.371	1.00	38.62	B	C
ATOM	8029	CB	ALA	282	112.795	77.301	16.792	1.00	37.75	B	C
ATOM	8030	C	ALA	282	112.863	76.619	14.403	1.00	37.34	B	C
ATOM	8031	O	ALA	282	111.797	76.463	13.815	1.00	36.86	B	O
ATOM	8032	N	THR	283	113.905	75.816	14.231	1.00	36.50	B	N
ATOM	8033	CA	THR	283	113.828	74.672	13.335	1.00	35.84	B	C
ATOM	8034	CB	THR	283	114.867	74.772	12.218	1.00	37.70	B	C
ATOM	8035	OG1	THR	283	114.665	75.994	11.495	1.00	41.71	B	O

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## FIG. 4 - 165

(Continued)

ATOM	8036	CG2	THR	283	114.736	73.595	11.265	1.00	37.32	B	C
ATOM	8037	C	THR	283	114.074	73.403	14.125	1.00	33.58	B	C
ATOM	8038	O	THR	283	115.098	73.263	14.774	1.00	34.31	B	O
ATOM	8039	N	SER	284	113.123	72.482	14.073	1.00	32.05	B	N
ATOM	8040	CA	SER	284	113.250	71.230	14.800	1.00	30.43	B	C
ATOM	8041	CB	SER	284	111.935	70.893	15.507	1.00	28.61	B	C
ATOM	8042	OG	SER	284	111.722	71.761	16.605	1.00	29.31	B	O
ATOM	8043	C	SER	284	113.638	70.090	13.883	1.00	30.34	B	C
ATOM	8044	O	SER	284	113.003	69.865	12.850	1.00	31.22	B	O
ATOM	8045	N	ILE	285	114.684	69.367	14.260	1.00	29.19	B	N
ATOM	8046	CA	ILE	285	115.130	68.241	13.457	1.00	28.80	B	C
ATOM	8047	CB	ILE	285	116.660	68.037	13.546	1.00	29.35	B	C
ATOM	8048	CG2	ILE	285	117.103	66.979	12.548	1.00	29.12	B	C
ATOM	8049	CG1	ILE	285	117.383	69.350	13.250	1.00	30.38	B	C
ATOM	8050	CD1	ILE	285	117.408	70.303	14.428	1.00	34.47	B	C
ATOM	8051	C	ILE	285	114.429	66.996	13.976	1.00	28.14	B	C
ATOM	8052	O	ILE	285	114.472	66.694	15.168	1.00	30.23	B	O
ATOM	8053	N	GLN	286	113.775	66.278	13.078	1.00	25.84	B	N
ATOM	8054	CA	GLN	286	113.067	65.076	13.457	1.00	24.81	B	C
ATOM	8055	CB	GLN	286	111.852	64.886	12.550	1.00	23.81	B	C
ATOM	8056	CG	GLN	286	111.169	63.547	12.715	1.00	23.29	B	C
ATOM	8057	CD	GLN	286	109.928	63.417	11.868	1.00	23.98	B	C
ATOM	8058	OE1	GLN	286	109.253	62.388	11.894	1.00	25.22	B	O
ATOM	8059	NE2	GLN	286	109.614	64.461	11.110	1.00	23.87	B	N
ATOM	8060	C	GLN	286	113.955	63.838	13.386	1.00	25.74	B	C
ATOM	8061	O	GLN	286	114.832	63.732	12.526	1.00	26.39	B	O
ATOM	8062	N	ILE	287	113.723	62.908	14.307	1.00	24.54	B	N
ATOM	8063	CA	ILE	287	114.458	61.655	14.346	1.00	23.40	B	C
ATOM	8064	CB	ILE	287	115.193	61.481	15.694	1.00	21.87	B	C
ATOM	8065	CG2	ILE	287	115.925	60.143	15.728	1.00	20.61	B	C
ATOM	8066	CG1	ILE	287	116.180	62.632	15.887	1.00	19.27	B	C
ATOM	8067	CD1	ILE	287	117.054	62.506	17.113	1.00	20.58	B	C
ATOM	8068	C	ILE	287	113.394	60.578	14.186	1.00	24.59	B	C
ATOM	8069	O	ILE	287	112.729	60.204	15.142	1.00	27.03	B	O
ATOM	8070	N	THR	288	113.219	60.093	12.966	1.00	25.43	B	N
ATOM	8071	CA	THR	288	112.205	59.088	12.708	1.00	26.10	B	C
ATOM	8072	CB	THR	288	111.964	58.927	11.188	1.00	26.69	B	C
ATOM	8073	OG1	THR	288	113.172	58.516	10.539	1.00	26.37	B	O
ATOM	8074	CG2	THR	288	111.510	60.255	10.593	1.00	25.25	B	C
ATOM	8075	C	THR	288	112.529	57.741	13.335	1.00	26.85	B	C
ATOM	8076	O	THR	288	113.687	57.379	13.503	1.00	27.04	B	O
ATOM	8077	N	ALA	289	111.484	57.011	13.702	1.00	28.37	B	N
ATOM	8078	CA	ALA	289	111.638	55.705	14.325	1.00	27.90	B	C
ATOM	8079	CB	ALA	289	110.271	55.151	14.710	1.00	26.91	B	C
ATOM	8080	C	ALA	289	112.348	54.740	13.380	1.00	27.44	B	C
ATOM	8081	O	ALA	289	112.550	55.038	12.205	1.00	28.30	B	O
ATOM	8082	N	PRO	290	112.758	53.577	13.895	1.00	26.01	B	N
ATOM	8083	CD	PRO	290	112.903	53.280	15.328	1.00	24.74	B	C
ATOM	8084	CA	PRO	290	113.445	52.569	13.089	1.00	25.29	B	C

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(Continued)

## FIG. 4 - 166

ATOM	8085	CB	PRO	290	113.949	51.587	14.138	1.00	25.76	B	C
ATOM	8086	CG	PRO	290	114.151	52.467	15.342	1.00	25.10	B	C
ATOM	8087	C	PRO	290	112.465	51.931	12.110	1.00	25.85	B	C
ATOM	8088	O	PRO	290	111.255	51.961	12.330	1.00	25.95	B	O
ATOM	8089	N	ALA	291	112.988	51.345	11.038	1.00	25.39	B	N
ATOM	8090	CA	ALA	291	112.143	50.730	10.024	1.00	26.17	B	C
ATOM	8091	CB	ALA	291	112.987	50.271	8.846	1.00	26.28	B	C
ATOM	8092	C	ALA	291	111.337	49.568	10.573	1.00	27.18	B	C
ATOM	8093	O	ALA	291	110.203	49.331	10.145	1.00	27.46	B	O
ATOM	8094	N	SER	292	111.916	48.843	11.521	1.00	27.54	B	N
ATOM	8095	CA	SER	292	111.220	47.704	12.103	1.00	28.19	B	C
ATOM	8096	CB	SER	292	112.161	46.892	12.993	1.00	28.00	B	C
ATOM	8097	OG	SER	292	112.525	47.626	14.145	1.00	32.22	B	O
ATOM	8098	C	SER	292	110.027	48.182	12.922	1.00	28.13	B	C
ATOM	8099	O	SER	292	109.176	47.376	13.307	1.00	29.52	B	O
ATOM	8100	N	MET	293	109.976	49.487	13.190	1.00	25.00	B	N
ATOM	8101	CA	MET	293	108.881	50.072	13.955	1.00	24.80	B	C
ATOM	8102	CB	MET	293	109.387	51.173	14.892	1.00	24.61	B	C
ATOM	8103	CG	MET	293	110.231	50.703	16.060	1.00	26.88	B	C
ATOM	8104	SD	MET	293	109.323	49.647	17.189	1.00	27.80	B	S
ATOM	8105	CE	MET	293	110.457	48.319	17.438	1.00	25.74	B	C
ATOM	8106	C	MET	293	107.836	50.677	13.027	1.00	24.57	B	C
ATOM	8107	O	MET	293	106.641	50.528	13.252	1.00	25.32	B	O
ATOM	8108	N	LEU	294	108.292	51.360	11.983	1.00	24.37	B	N
ATOM	8109	CA	LEU	294	107.393	52.008	11.041	1.00	23.80	B	C
ATOM	8110	CB	LEU	294	108.183	52.930	10.114	1.00	23.40	B	C
ATOM	8111	CG	LEU	294	108.945	54.072	10.786	1.00	24.87	B	C
ATOM	8112	CD1	LEU	294	109.806	54.787	9.758	1.00	22.08	B	C
ATOM	8113	CD2	LEU	294	107.958	55.037	11.440	1.00	23.08	B	C
ATOM	8114	C	LEU	294	106.540	51.059	10.204	1.00	23.95	B	C
ATOM	8115	O	LEU	294	105.714	51.510	9.422	1.00	25.36	B	O
ATOM	8116	N	ILE	295	106.724	49.754	10.357	1.00	23.92	B	N
ATOM	8117	CA	ILE	295	105.923	48.812	9.580	1.00	25.26	B	C
ATOM	8118	CB	ILE	295	106.601	47.444	9.453	1.00	26.06	B	C
ATOM	8119	CG2	ILE	295	107.972	47.595	8.812	1.00	26.54	B	C
ATOM	8120	CG1	ILE	295	106.698	46.796	10.831	1.00	24.44	B	C
ATOM	8121	CD1	ILE	295	107.211	45.388	10.789	1.00	28.37	B	C
ATOM	8122	C	ILE	295	104.564	48.575	10.221	1.00	26.01	B	C
ATOM	8123	O	ILE	295	103.805	47.712	9.775	1.00	28.75	B	O
ATOM	8124	N	GLY	296	104.263	49.328	11.273	1.00	24.77	B	N
ATOM	8125	CA	GLY	296	102.992	49.167	11.951	1.00	22.28	B	C
ATOM	8126	C	GLY	296	102.908	50.040	13.182	1.00	21.29	B	C
ATOM	8127	O	GLY	296	103.820	50.818	13.447	1.00	20.80	B	O
ATOM	8128	N	ASP	297	101.818	49.920	13.935	1.00	20.38	B	N
ATOM	8129	CA	ASP	297	101.654	50.718	15.141	1.00	20.14	B	C
ATOM	8130	CB	ASP	297	100.366	50.339	15.874	1.00	21.58	B	C
ATOM	8131	CG	ASP	297	99.109	50.665	15.078	1.00	22.60	B	C
ATOM	8132	OD1	ASP	297	98.016	50.234	15.502	1.00	25.00	B	O
ATOM	8133	OD2	ASP	297	99.200	51.350	14.041	1.00	22.18	B	O

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## FIG. 4 - 167

(Continued)

ATOM	8134	C	ASP	297	102.845	50.481	16.065	1.00	20.31	B	C
ATOM	8135	O	ASP	297	103.419	49.390	16.096	1.00	20.82	B	O
ATOM	8136	N	HIS	298	103.220	51.508	16.814	1.00	16.87	B	N
ATOM	8137	CA	HIS	298	104.335	51.384	17.734	1.00	16.48	B	C
ATOM	8138	CB	HIS	298	105.669	51.399	16.968	1.00	14.91	B	C
ATOM	8139	CG	HIS	298	105.868	52.628	16.137	1.00	12.24	B	C
ATOM	8140	CD2	HIS	298	106.539	53.775	16.391	1.00	10.39	B	C
ATOM	8141	ND1	HIS	298	105.264	52.802	14.909	1.00	11.35	B	N
ATOM	8142	CE1	HIS	298	105.551	54.005	14.445	1.00	11.25	B	C
ATOM	8143	NE2	HIS	298	106.323	54.616	15.326	1.00	11.96	B	N
ATOM	8144	C	HIS	298	104.274	52.560	18.693	1.00	15.84	B	C
ATOM	8145	O	HIS	298	103.484	53.476	18.505	1.00	17.04	B	O
ATOM	8146	N	TYR	299	105.127	52.539	19.706	1.00	15.50	B	N
ATOM	8147	CA	TYR	299	105.163	53.599	20.698	1.00	15.35	B	C
ATOM	8148	CB	TYR	299	104.640	53.095	22.047	1.00	14.51	B	C
ATOM	8149	CG	TYR	299	103.343	52.320	22.037	1.00	14.30	B	C
ATOM	8150	CD1	TYR	299	102.120	52.973	21.942	1.00	13.49	B	C
ATOM	8151	CE1	TYR	299	100.924	52.269	22.019	1.00	15.63	B	C
ATOM	8152	CD2	TYR	299	103.341	50.933	22.198	1.00	14.56	B	C
ATOM	8153	CE2	TYR	299	102.150	50.216	22.273	1.00	15.40	B	C
ATOM	8154	CZ	TYR	299	100.943	50.891	22.186	1.00	15.73	B	C
ATOM	8155	OH	TYR	299	99.756	50.197	22.286	1.00	15.37	B	O
ATOM	8156	C	TYR	299	106.583	54.084	20.952	1.00	16.54	B	C
ATOM	8157	O	TYR	299	107.559	53.364	20.732	1.00	15.53	B	O
ATOM	8158	N	LEU	300	106.688	55.316	21.428	1.00	16.67	B	N
ATOM	8159	CA	LEU	300	107.975	55.853	21.818	1.00	17.75	B	C
ATOM	8160	CB	LEU	300	107.986	57.367	21.654	1.00	18.54	B	C
ATOM	8161	CG	LEU	300	109.238	58.059	22.183	1.00	20.06	B	C
ATOM	8162	CD1	LEU	300	110.449	57.535	21.429	1.00	20.50	B	C
ATOM	8163	CD2	LEU	300	109.107	59.567	22.024	1.00	20.10	B	C
ATOM	8164	C	LEU	300	107.897	55.477	23.294	1.00	18.55	B	C
ATOM	8165	O	LEU	300	106.894	55.783	23.935	1.00	20.71	B	O
ATOM	8166	N	CYS	301	108.901	54.805	23.849	1.00	18.50	B	N
ATOM	8167	CA	CYS	301	108.788	54.418	25.252	1.00	20.22	B	C
ATOM	8168	CB	CYS	301	108.582	52.907	25.375	1.00	20.55	B	C
ATOM	8169	SG	CYS	301	109.922	51.905	24.722	1.00	26.11	B	S
ATOM	8170	C	CYS	301	109.895	54.842	26.194	1.00	20.82	B	C
ATOM	8171	O	CYS	301	109.816	54.579	27.395	1.00	21.62	B	O
ATOM	8172	N	ASP	302	110.922	55.496	25.662	1.00	22.13	B	N
ATOM	8173	CA	ASP	302	112.035	55.968	26.481	1.00	20.03	B	C
ATOM	8174	CB	ASP	302	112.875	54.810	27.014	1.00	20.49	B	C
ATOM	8175	CG	ASP	302	114.035	55.296	27.868	1.00	25.77	B	C
ATOM	8176	OD1	ASP	302	113.880	55.344	29.109	1.00	26.02	B	O
ATOM	8177	OD2	ASP	302	115.097	55.664	27.297	1.00	27.73	B	O
ATOM	8178	C	ASP	302	112.959	56.894	25.711	1.00	20.08	B	C
ATOM	8179	O	ASP	302	113.367	56.596	24.586	1.00	19.30	B	O
ATOM	8180	N	VAL	303	113.302	58.010	26.343	1.00	20.41	B	N
ATOM	8181	CA	VAL	303	114.188	59.000	25.756	1.00	20.36	B	C
ATOM	8182	CB	VAL	303	113.435	60.316	25.470	1.00	19.97	B	C

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(Continued)

## FIG. 4 - 1 6 8

ATOM	8183	CG1	VAL	303	114.387	61.347	24.857	1.00	20.23	B	C
ATOM	8184	CG2	VAL	303	112.260	60.043	24.540	1.00	17.52	B	C
ATOM	8185	C	VAL	303	115.267	59.251	26.788	1.00	21.02	B	C
ATOM	8186	O	VAL	303	114.950	59.568	27.939	1.00	19.39	B	O
ATOM	8187	N	THR	304	116.536	59.112	26.389	1.00	21.38	B	N
ATOM	8188	CA	THR	304	117.639	59.313	27.332	1.00	21.48	B	C
ATOM	8189	CB	THR	304	118.008	58.002	28.046	1.00	19.77	B	C
ATOM	8190	OG1	THR	304	116.869	57.496	28.751	1.00	19.55	B	O
ATOM	8191	CG2	THR	304	119.136	58.242	29.026	1.00	20.57	B	C
ATOM	8192	C	THR	304	118.925	59.851	26.729	1.00	22.96	B	C
ATOM	8193	O	THR	304	119.579	59.159	25.952	1.00	25.30	B	O
ATOM	8194	N	TRP	305	119.307	61.069	27.102	1.00	22.41	B	N
ATOM	8195	CA	TRP	305	120.545	61.643	26.583	1.00	21.86	B	C
ATOM	8196	CB	TRP	305	120.696	63.114	26.975	1.00	20.21	B	C
ATOM	8197	CG	TRP	305	119.682	64.002	26.354	1.00	18.90	B	C
ATOM	8198	CD2	TRP	305	119.834	64.751	25.150	1.00	18.79	B	C
ATOM	8199	CE2	TRP	305	118.614	65.413	24.917	1.00	20.14	B	C
ATOM	8200	CE3	TRP	305	120.885	64.928	24.243	1.00	18.65	B	C
ATOM	8201	CD1	TRP	305	118.414	64.232	26.794	1.00	17.49	B	C
ATOM	8202	NE1	TRP	305	117.764	65.077	25.938	1.00	18.37	B	N
ATOM	8203	CZ2	TRP	305	118.413	66.242	23.812	1.00	19.16	B	C
ATOM	8204	CZ3	TRP	305	120.689	65.746	23.152	1.00	19.59	B	C
ATOM	8205	CH2	TRP	305	119.459	66.395	22.943	1.00	21.43	B	C
ATOM	8206	C	TRP	305	121.722	60.875	27.148	1.00	22.21	B	C
ATOM	8207	O	TRP	305	121.743	60.552	28.338	1.00	21.63	B	O
ATOM	8208	N	ALA	306	122.697	60.591	26.285	1.00	22.53	B	N
ATOM	8209	CA	ALA	306	123.899	59.864	26.673	1.00	21.31	B	C
ATOM	8210	CB	ALA	306	124.350	58.969	25.533	1.00	20.65	B	C
ATOM	8211	C	ALA	306	124.975	60.882	27.000	1.00	21.97	B	C
ATOM	8212	O	ALA	306	125.675	60.767	28.007	1.00	20.32	B	O
ATOM	8213	N	THR	307	125.086	61.885	26.133	1.00	23.85	B	N
ATOM	8214	CA	THR	307	126.057	62.964	26.284	1.00	24.42	B	C
ATOM	8215	CB	THR	307	127.285	62.744	25.411	1.00	22.67	B	C
ATOM	8216	OG1	THR	307	126.894	62.855	24.040	1.00	25.33	B	O
ATOM	8217	CG2	THR	307	127.892	61.374	25.659	1.00	19.34	B	C
ATOM	8218	C	THR	307	125.397	64.250	25.812	1.00	25.73	B	C
ATOM	8219	O	THR	307	124.177	64.326	25.731	1.00	28.17	B	O
ATOM	8220	N	GLN	308	126.210	65.249	25.479	1.00	26.09	B	N
ATOM	8221	CA	GLN	308	125.699	66.540	25.022	1.00	24.49	B	C
ATOM	8222	CB	GLN	308	126.762	67.634	25.175	1.00	22.95	B	C
ATOM	8223	CG	GLN	308	127.301	67.811	26.574	1.00	21.20	B	C
ATOM	8224	CD	GLN	308	126.256	68.296	27.548	1.00	20.30	B	C
ATOM	8225	OE1	GLN	308	126.477	68.290	28.754	1.00	23.08	B	O
ATOM	8226	NE2	GLN	308	125.116	68.727	27.032	1.00	21.02	B	N
ATOM	8227	C	GLN	308	125.284	66.501	23.569	1.00	25.09	B	C
ATOM	8228	O	GLN	308	124.612	67.411	23.095	1.00	26.23	B	O
ATOM	8229	N	GLU	309	125.687	65.459	22.855	1.00	25.59	B	N
ATOM	8230	CA	GLU	309	125.370	65.374	21.440	1.00	26.16	B	C
ATOM	8231	CB	GLU	309	126.581	65.807	20.627	1.00	25.99	B	C

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## FIG. 4 - 169

(Continued)

ATOM	8232	CG	GLU	309	126.925	67.280	20.774	1.00	29.27	B	C
ATOM	8233	CD	GLU	309	128.243	67.637	20.109	1.00	31.48	B	C
ATOM	8234	OE1	GLU	309	128.614	66.968	19.115	1.00	33.35	B	O
ATOM	8235	OE2	GLU	309	128.900	68.593	20.572	1.00	32.54	B	O
ATOM	8236	C	GLU	309	124.939	63.991	21.004	1.00	26.83	B	C
ATOM	8237	O	GLU	309	124.850	63.712	19.806	1.00	28.64	B	O
ATOM	8238	N	ARG	310	124.674	63.131	21.982	1.00	25.93	B	N
ATOM	8239	CA	ARG	310	124.246	61.765	21.723	1.00	24.07	B	C
ATOM	8240	CB	ARG	310	125.357	60.790	22.121	1.00	24.28	B	C
ATOM	8241	CG	ARG	310	125.012	59.317	21.952	1.00	25.64	B	C
ATOM	8242	CD	ARG	310	126.255	58.469	22.132	1.00	24.20	B	C
ATOM	8243	NE	ARG	310	127.225	58.790	21.097	1.00	25.36	B	N
ATOM	8244	CZ	ARG	310	128.533	58.590	21.195	1.00	26.41	B	C
ATOM	8245	NH1	ARG	310	129.056	58.063	22.298	1.00	26.17	B	N
ATOM	8246	NH2	ARG	310	129.321	58.928	20.183	1.00	26.60	B	N
ATOM	8247	C	ARG	310	122.984	61.488	22.528	1.00	23.55	B	C
ATOM	8248	O	ARG	310	122.965	61.607	23.757	1.00	23.67	B	O
ATOM	8249	N	ILE	311	121.922	61.124	21.829	1.00	21.75	B	N
ATOM	8250	CA	ILE	311	120.663	60.843	22.491	1.00	20.40	B	C
ATOM	8251	CB	ILE	311	119.586	61.876	22.067	1.00	18.52	B	C
ATOM	8252	CG2	ILE	311	119.293	61.742	20.593	1.00	18.77	B	C
ATOM	8253	CG1	ILE	311	118.305	61.686	22.879	1.00	18.16	B	C
ATOM	8254	CD1	ILE	311	117.255	62.774	22.626	1.00	15.33	B	C
ATOM	8255	C	ILE	311	120.233	59.440	22.107	1.00	20.81	B	C
ATOM	8256	O	ILE	311	120.380	59.036	20.959	1.00	21.43	B	O
ATOM	8257	N	SER	312	119.734	58.686	23.080	1.00	21.54	B	N
ATOM	8258	CA	SER	312	119.269	57.326	22.832	1.00	21.49	B	C
ATOM	8259	CB	SER	312	119.889	56.355	23.837	1.00	22.73	B	C
ATOM	8260	OG	SER	312	119.365	56.575	25.132	1.00	23.02	B	O
ATOM	8261	C	SER	312	117.758	57.315	22.985	1.00	20.72	B	C
ATOM	8262	O	SER	312	117.214	57.998	23.853	1.00	22.17	B	O
ATOM	8263	N	LEU	313	117.088	56.544	22.136	1.00	21.93	B	N
ATOM	8264	CA	LEU	313	115.631	56.428	22.155	1.00	22.17	B	C
ATOM	8265	CB	LEU	313	115.013	57.179	20.979	1.00	23.76	B	C
ATOM	8266	CG	LEU	313	115.314	58.656	20.754	1.00	27.56	B	C
ATOM	8267	CD1	LEU	313	114.707	59.068	19.410	1.00	29.23	B	C
ATOM	8268	CD2	LEU	313	114.740	59.497	21.890	1.00	28.89	B	C
ATOM	8269	C	LEU	313	115.229	54.968	22.022	1.00	22.50	B	C
ATOM	8270	O	LEU	313	115.868	54.209	21.293	1.00	22.55	B	O
ATOM	8271	N	GLN	314	114.167	54.579	22.722	1.00	22.54	B	N
ATOM	8272	CA	GLN	314	113.666	53.216	22.639	1.00	23.08	B	C
ATOM	8273	CB	GLN	314	113.682	52.549	24.012	1.00	22.45	B	C
ATOM	8274	CG	GLN	314	115.065	52.459	24.626	1.00	25.62	B	C
ATOM	8275	CD	GLN	314	115.092	51.630	25.898	1.00	26.36	B	C
ATOM	8276	OE1	GLN	314	114.835	50.428	25.870	1.00	27.68	B	O
ATOM	8277	NE2	GLN	314	115.403	52.273	27.023	1.00	25.65	B	N
ATOM	8278	C	GLN	314	112.242	53.240	22.083	1.00	23.35	B	C
ATOM	8279	O	GLN	314	111.412	54.045	22.513	1.00	22.96	B	O
ATOM	8280	N	TRP	315	111.984	52.372	21.108	1.00	22.35	B	N

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(Continued)

## FIG. 4 - 170

ATOM	8281	CA	TRP	315	110.672	52.262	20.484	1.00	21.75	B	C
ATOM	8282	CB	TRP	315	110.769	52.440	18.968	1.00	21.09	B	C
ATOM	8283	CG	TRP	315	111.376	53.741	18.540	1.00	21.09	B	C
ATOM	8284	CD2	TRP	315	110.678	54.940	18.176	1.00	19.81	B	C
ATOM	8285	CE2	TRP	315	111.654	55.901	17.824	1.00	20.24	B	C
ATOM	8286	CE3	TRP	315	109.325	55.295	18.113	1.00	17.16	B	C
ATOM	8287	CD1	TRP	315	112.705	54.018	18.405	1.00	21.12	B	C
ATOM	8288	NE1	TRP	315	112.880	55.310	17.974	1.00	21.84	B	N
ATOM	8289	CZ2	TRP	315	111.321	57.197	17.413	1.00	18.97	B	C
ATOM	8290	CZ3	TRP	315	108.992	56.588	17.704	1.00	20.13	B	C
ATOM	8291	CH2	TRP	315	109.990	57.522	17.359	1.00	19.26	B	C
ATOM	8292	C	TRP	315	110.118	50.880	20.790	1.00	22.37	B	C
ATOM	8293	O	TRP	315	110.877	49.922	20.941	1.00	24.80	B	O
ATOM	8294	N	LEU	316	108.799	50.772	20.872	1.00	21.02	B	N
ATOM	8295	CA	LEU	316	108.159	49.502	21.184	1.00	20.90	B	C
ATOM	8296	CB	LEU	316	107.653	49.544	22.628	1.00	19.84	B	C
ATOM	8297	CG	LEU	316	106.866	48.358	23.194	1.00	19.46	B	C
ATOM	8298	CD1	LEU	316	107.786	47.157	23.408	1.00	18.22	B	C
ATOM	8299	CD2	LEU	316	106.223	48.783	24.501	1.00	16.50	B	C
ATOM	8300	C	LEU	316	106.995	49.228	20.229	1.00	20.90	B	C
ATOM	8301	O	LEU	316	106.161	50.098	20.000	1.00	22.41	B	O
ATOM	8302	N	ARG	317	106.941	48.026	19.666	1.00	19.89	B	N
ATOM	8303	CA	ARG	317	105.851	47.678	18.753	1.00	20.30	B	C
ATOM	8304	CB	ARG	317	106.154	46.362	18.035	1.00	20.73	B	C
ATOM	8305	CG	ARG	317	107.248	46.480	16.993	1.00	23.49	B	C
ATOM	8306	CD	ARG	317	107.524	45.149	16.321	1.00	24.95	B	C
ATOM	8307	NE	ARG	317	108.347	45.314	15.128	1.00	25.57	B	N
ATOM	8308	CZ	ARG	317	108.925	44.313	14.476	1.00	26.73	B	C
ATOM	8309	NH1	ARG	317	108.775	43.061	14.897	1.00	23.81	B	N
ATOM	8310	NH2	ARG	317	109.656	44.567	13.401	1.00	29.12	B	N
ATOM	8311	C	ARG	317	104.537	47.545	19.512	1.00	19.31	B	C
ATOM	8312	O	ARG	317	104.541	47.266	20.713	1.00	17.59	B	O
ATOM	8313	N	ARG	318	103.415	47.747	18.820	1.00	18.54	B	N
ATOM	8314	CA	ARG	318	102.117	47.621	19.476	1.00	17.04	B	C
ATOM	8315	CB	ARG	318	100.970	47.781	18.483	1.00	17.09	B	C
ATOM	8316	CG	ARG	318	99.608	47.794	19.164	1.00	17.74	B	C
ATOM	8317	CD	ARG	318	98.613	48.660	18.414	1.00	16.48	B	C
ATOM	8318	NE	ARG	318	97.326	48.672	19.092	1.00	16.05	B	N
ATOM	8319	CZ	ARG	318	96.320	49.478	18.771	1.00	17.02	B	C
ATOM	8320	NH1	ARG	318	96.464	50.342	17.771	1.00	13.59	B	N
ATOM	8321	NH2	ARG	318	95.180	49.428	19.460	1.00	12.42	B	N
ATOM	8322	C	ARG	318	102.085	46.251	20.132	1.00	15.28	B	C
ATOM	8323	O	ARG	318	101.569	46.103	21.234	1.00	15.74	B	O
ATOM	8324	N	ILE	319	102.627	45.251	19.440	1.00	15.27	B	N
ATOM	8325	CA	ILE	319	102.757	43.912	20.007	1.00	15.37	B	C
ATOM	8326	CB	ILE	319	103.006	42.848	18.949	1.00	15.60	B	C
ATOM	8327	CG2	ILE	319	103.268	41.519	19.621	1.00	17.64	B	C
ATOM	8328	CG1	ILE	319	101.793	42.732	18.036	1.00	15.37	B	C
ATOM	8329	CD1	ILE	319	100.524	42.425	18.781	1.00	15.54	B	C

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## FIG. 4 - 171

(Continued)

ATOM	8330	C	ILE	319	104.036	44.122	20.802	1.00	16.78	B	C
ATOM	8331	O	ILE	319	105.145	44.086	20.257	1.00	16.37	B	O
ATOM	8332	N	GLN	320	103.850	44.367	22.092	1.00	17.82	B	N
ATOM	8333	CA	GLN	320	104.923	44.693	23.016	1.00	18.01	B	C
ATOM	8334	CB	GLN	320	104.293	45.341	24.248	1.00	16.84	B	C
ATOM	8335	CG	GLN	320	103.383	46.495	23.863	1.00	16.48	B	C
ATOM	8336	CD	GLN	320	102.833	47.250	25.048	1.00	17.06	B	C
ATOM	8337	OE1	GLN	320	103.544	47.509	26.016	1.00	18.02	B	O
ATOM	8338	NE2	GLN	320	101.566	47.633	24.966	1.00	16.46	B	N
ATOM	8339	C	GLN	320	105.964	43.663	23.437	1.00	18.97	B	C
ATOM	8340	O	GLN	320	106.399	43.654	24.594	1.00	20.18	B	O
ATOM	8341	N	ASN	321	106.382	42.800	22.520	1.00	19.64	B	N
ATOM	8342	CA	ASN	321	107.420	41.846	22.875	1.00	21.44	B	C
ATOM	8343	CB	ASN	321	106.950	40.399	22.719	1.00	23.79	B	C
ATOM	8344	CG	ASN	321	106.409	40.085	21.332	1.00	27.68	B	C
ATOM	8345	OD1	ASN	321	106.593	40.839	20.374	1.00	28.16	B	O
ATOM	8346	ND2	ASN	321	105.745	38.934	21.255	1.00	30.91	B	N
ATOM	8347	C	ASN	321	108.658	42.087	22.036	1.00	21.63	B	C
ATOM	8348	O	ASN	321	109.533	41.228	21.940	1.00	23.87	B	O
ATOM	8349	N	TYR	322	108.735	43.275	21.444	1.00	20.56	B	N
ATOM	8350	CA	TYR	322	109.873	43.644	20.613	1.00	18.63	B	C
ATOM	8351	CB	TYR	322	109.605	43.208	19.178	1.00	18.95	B	C
ATOM	8352	CG	TYR	322	110.766	43.362	18.228	1.00	21.29	B	C
ATOM	8353	CD1	TYR	322	111.086	44.604	17.677	1.00	21.18	B	C
ATOM	8354	CE1	TYR	322	112.118	44.733	16.759	1.00	22.17	B	C
ATOM	8355	CD2	TYR	322	111.520	42.252	17.840	1.00	20.55	B	C
ATOM	8356	CE2	TYR	322	112.557	42.372	16.925	1.00	21.33	B	C
ATOM	8357	CZ	TYR	322	112.847	43.611	16.387	1.00	22.88	B	C
ATOM	8358	OH	TYR	322	113.855	43.726	15.461	1.00	28.00	B	O
ATOM	8359	C	TYR	322	110.115	45.149	20.678	1.00	18.95	B	C
ATOM	8360	O	TYR	322	109.240	45.945	20.338	1.00	20.45	B	O
ATOM	8361	N	SER	323	111.299	45.537	21.139	1.00	18.50	B	N
ATOM	8362	CA	SER	323	111.657	46.946	21.233	1.00	17.89	B	C
ATOM	8363	CB	SER	323	111.623	47.418	22.684	1.00	18.88	B	C
ATOM	8364	OG	SER	323	112.602	46.740	23.444	1.00	21.21	B	O
ATOM	8365	C	SER	323	113.057	47.131	20.677	1.00	16.99	B	C
ATOM	8366	O	SER	323	113.851	46.190	20.657	1.00	15.79	B	O
ATOM	8367	N	VAL	324	113.360	48.345	20.230	1.00	16.51	B	N
ATOM	8368	CA	VAL	324	114.672	48.638	19.664	1.00	17.39	B	C
ATOM	8369	CB	VAL	324	114.612	48.684	18.126	1.00	18.70	B	C
ATOM	8370	CG1	VAL	324	113.454	49.550	17.692	1.00	22.04	B	C
ATOM	8371	CG2	VAL	324	115.901	49.257	17.565	1.00	20.08	B	C
ATOM	8372	C	VAL	324	115.201	49.970	20.151	1.00	16.54	B	C
ATOM	8373	O	VAL	324	114.460	50.946	20.243	1.00	19.05	B	O
ATOM	8374	N	MET	325	116.487	50.011	20.463	1.00	15.89	B	N
ATOM	8375	CA	MET	325	117.104	51.243	20.914	1.00	16.61	B	C
ATOM	8376	CB	MET	325	118.053	50.997	22.083	1.00	17.97	B	C
ATOM	8377	CG	MET	325	118.682	52.280	22.597	1.00	19.56	B	C
ATOM	8378	SD	MET	325	119.851	52.014	23.915	1.00	22.61	B	S

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(Continued)

## FIG. 4 - 172

ATOM	8379	CE	MET	325	118.765	51.442	25.211	1.00	21.39	B	C
ATOM	8380	C	MET	325	117.895	51.875	19.782	1.00	17.82	B	C
ATOM	8381	O	MET	325	118.658	51.198	19.082	1.00	15.28	B	O
ATOM	8382	N	ASP	326	117.698	53.175	19.607	1.00	18.85	B	N
ATOM	8383	CA	ASP	326	118.409	53.922	18.591	1.00	21.89	B	C
ATOM	8384	CB	ASP	326	117.436	54.685	17.695	1.00	22.04	B	C
ATOM	8385	CG	ASP	326	117.533	54.272	16.244	1.00	23.15	B	C
ATOM	8386	OD1	ASP	326	116.800	54.855	15.418	1.00	25.35	B	O
ATOM	8387	OD2	ASP	326	118.334	53.366	15.922	1.00	23.67	B	O
ATOM	8388	C	ASP	326	119.299	54.904	19.327	1.00	24.54	B	C
ATOM	8389	O	ASP	326	118.896	55.494	20.335	1.00	25.63	B	O
ATOM	8390	N	ILE	327	120.521	55.062	18.842	1.00	25.49	B	N
ATOM	8391	CA	ILE	327	121.451	55.986	19.459	1.00	27.44	B	C
ATOM	8392	CB	ILE	327	122.713	55.263	19.936	1.00	27.10	B	C
ATOM	8393	CG2	ILE	327	123.697	56.264	20.515	1.00	27.85	B	C
ATOM	8394	CG1	ILE	327	122.321	54.221	20.984	1.00	25.49	B	C
ATOM	8395	CD1	ILE	327	123.476	53.506	21.594	1.00	27.60	B	C
ATOM	8396	C	ILE	327	121.784	57.005	18.395	1.00	29.15	B	C
ATOM	8397	O	ILE	327	122.357	56.673	17.357	1.00	31.19	B	O
ATOM	8398	N	CYS	328	121.414	58.250	18.653	1.00	30.14	B	N
ATOM	8399	CA	CYS	328	121.624	59.298	17.684	1.00	31.56	B	C
ATOM	8400	C	CYS	328	122.624	60.356	18.084	1.00	32.64	B	C
ATOM	8401	O	CYS	328	122.525	60.972	19.153	1.00	33.03	B	O
ATOM	8402	CB	CYS	328	120.286	59.938	17.366	1.00	32.73	B	C
ATOM	8403	SG	CYS	328	118.979	58.689	17.154	1.00	36.31	B	S
ATOM	8404	N	ASP	329	123.596	60.555	17.200	1.00	32.72	B	N
ATOM	8405	CA	ASP	329	124.639	61.542	17.406	1.00	32.74	B	C
ATOM	8406	CB	ASP	329	125.997	60.975	16.981	1.00	34.70	B	C
ATOM	8407	CG	ASP	329	126.480	59.858	17.894	1.00	36.73	B	C
ATOM	8408	OD1	ASP	329	127.643	59.431	17.735	1.00	38.23	B	O
ATOM	8409	OD2	ASP	329	125.706	59.405	18.767	1.00	36.00	B	O
ATOM	8410	C	ASP	329	124.320	62.781	16.588	1.00	31.70	B	C
ATOM	8411	O	ASP	329	123.767	62.692	15.494	1.00	30.70	B	O
ATOM	8412	N	TYR	330	124.662	63.940	17.129	1.00	31.69	B	N
ATOM	8413	CA	TYR	330	124.420	65.191	16.428	1.00	33.40	B	C
ATOM	8414	CB	TYR	330	124.376	66.354	17.411	1.00	30.81	B	C
ATOM	8415	CG	TYR	330	124.322	67.693	16.728	1.00	29.75	B	C
ATOM	8416	CD1	TYR	330	123.185	68.089	16.030	1.00	30.07	B	C
ATOM	8417	CE1	TYR	330	123.121	69.326	15.399	1.00	30.94	B	C
ATOM	8418	CD2	TYR	330	125.407	68.568	16.777	1.00	30.62	B	C
ATOM	8419	CE2	TYR	330	125.356	69.814	16.150	1.00	30.16	B	C
ATOM	8420	CZ	TYR	330	124.206	70.186	15.465	1.00	31.10	B	C
ATOM	8421	OH	TYR	330	124.122	71.422	14.867	1.00	29.92	B	O
ATOM	8422	C	TYR	330	125.523	65.462	15.412	1.00	35.09	B	C
ATOM	8423	O	TYR	330	126.692	65.552	15.772	1.00	36.29	B	O
ATOM	8424	N	ASP	331	125.149	65.600	14.146	1.00	37.07	B	N
ATOM	8425	CA	ASP	331	126.123	65.886	13.106	1.00	39.50	B	C
ATOM	8426	CB	ASP	331	125.611	65.391	11.756	1.00	39.77	B	C
ATOM	8427	CG	ASP	331	126.665	65.464	10.677	1.00	40.31	B	C

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## FIG. 4 - 173

(Continued)

ATOM	8428	OD1	ASP	331	126.387	65.018	9.543	1.00	41.37	B	O
ATOM	8429	OD2	ASP	331	127.770	65.966	10.967	1.00	40.07	B	O
ATOM	8430	C	ASP	331	126.355	67.395	13.062	1.00	41.15	B	C
ATOM	8431	O	ASP	331	125.641	68.126	12.380	1.00	40.39	B	O
ATOM	8432	N	GLU	332	127.358	67.852	13.802	1.00	44.16	B	N
ATOM	8433	CA	GLU	332	127.690	69.271	13.879	1.00	47.17	B	C
ATOM	8434	CB	GLU	332	129.001	69.457	14.646	1.00	48.80	B	C
ATOM	8435	CG	GLU	332	129.367	70.901	14.922	1.00	51.70	B	C
ATOM	8436	CD	GLU	332	130.451	71.028	15.979	1.00	54.56	B	C
ATOM	8437	OE1	GLU	332	130.203	70.623	17.136	1.00	55.51	B	O
ATOM	8438	OE2	GLU	332	131.552	71.528	15.658	1.00	56.11	B	O
ATOM	8439	C	GLU	332	127.791	69.941	12.517	1.00	47.83	B	C
ATOM	8440	O	GLU	332	127.518	71.130	12.383	1.00	48.20	B	O
ATOM	8441	N	SER	333	128.179	69.175	11.505	1.00	48.69	B	N
ATOM	8442	CA	SER	333	128.312	69.715	10.161	1.00	49.93	B	C
ATOM	8443	CB	SER	333	129.246	68.835	9.327	1.00	50.95	B	C
ATOM	8444	OG	SER	333	130.521	68.723	9.943	1.00	54.48	B	O
ATOM	8445	C	SER	333	126.957	69.809	9.483	1.00	49.97	B	C
ATOM	8446	O	SER	333	126.514	70.893	9.108	1.00	50.95	B	O
ATOM	8447	N	SER	334	126.302	68.665	9.326	1.00	50.21	B	N
ATOM	8448	CA	SER	334	124.993	68.609	8.687	1.00	49.04	B	C
ATOM	8449	CB	SER	334	124.582	67.154	8.451	1.00	50.46	B	C
ATOM	8450	OG	SER	334	123.275	67.076	7.905	1.00	52.36	B	O
ATOM	8451	C	SER	334	123.934	69.288	9.536	1.00	47.42	B	C
ATOM	8452	O	SER	334	122.917	69.742	9.021	1.00	48.45	B	O
ATOM	8453	N	GLY	335	124.177	69.353	10.840	1.00	45.55	B	N
ATOM	8454	CA	GLY	335	123.219	69.965	11.738	1.00	42.54	B	C
ATOM	8455	C	GLY	335	122.081	69.007	12.033	1.00	40.97	B	C
ATOM	8456	O	GLY	335	121.179	69.318	12.807	1.00	40.87	B	O
ATOM	8457	N	ARG	336	122.117	67.834	11.409	1.00	38.61	B	N
ATOM	8458	CA	ARG	336	121.076	66.843	11.622	1.00	37.65	B	C
ATOM	8459	CB	ARG	336	120.725	66.143	10.306	1.00	39.07	B	C
ATOM	8460	CG	ARG	336	120.460	67.099	9.151	1.00	41.95	B	C
ATOM	8461	CD	ARG	336	119.339	66.597	8.248	1.00	45.61	B	C
ATOM	8462	NE	ARG	336	118.019	67.002	8.729	1.00	48.18	B	N
ATOM	8463	CZ	ARG	336	117.522	68.233	8.613	1.00	49.86	B	C
ATOM	8464	NH1	ARG	336	118.229	69.194	8.025	1.00	50.51	B	N
ATOM	8465	NH2	ARG	336	116.317	68.510	9.094	1.00	50.56	B	N
ATOM	8466	C	ARG	336	121.524	65.817	12.654	1.00	35.64	B	C
ATOM	8467	O	ARG	336	122.629	65.900	13.181	1.00	35.91	B	O
ATOM	8468	N	TRP	337	120.649	64.865	12.955	1.00	33.09	B	N
ATOM	8469	CA	TRP	337	120.955	63.818	13.918	1.00	30.08	B	C
ATOM	8470	CB	TRP	337	119.922	63.793	15.053	1.00	24.67	B	C
ATOM	8471	CG	TRP	337	119.993	64.979	15.954	1.00	20.03	B	C
ATOM	8472	CD2	TRP	337	120.670	65.059	17.214	1.00	17.75	B	C
ATOM	8473	CE2	TRP	337	120.550	66.390	17.671	1.00	17.16	B	C
ATOM	8474	CE3	TRP	337	121.374	64.137	17.997	1.00	15.36	B	C
ATOM	8475	CD1	TRP	337	119.498	66.224	15.709	1.00	19.73	B	C
ATOM	8476	NE1	TRP	337	119.827	67.079	16.736	1.00	18.61	B	N

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## FIG. 4 - 174

(Continued)

ATOM	8477	CZ2	TRP	337	121.110	66.825	18.875	1.00	18.08	B	C
ATOM	8478	CZ3	TRP	337	121.932	64.567	19.196	1.00	15.24	B	C
ATOM	8479	CH2	TRP	337	121.798	65.900	19.622	1.00	16.71	B	C
ATOM	8480	C	TRP	337	120.940	62.487	13.188	1.00	31.57	B	C
ATOM	8481	O	TRP	337	119.983	62.167	12.482	1.00	33.23	B	O
ATOM	8482	N	ASN	338	122.003	61.712	13.347	1.00	32.12	B	N
ATOM	8483	CA	ASN	338	122.079	60.426	12.691	1.00	33.02	B	C
ATOM	8484	CB	ASN	338	123.240	60.416	11.698	1.00	34.88	B	C
ATOM	8485	CG	ASN	338	122.957	61.271	10.471	1.00	38.68	B	C
ATOM	8486	OD1	ASN	338	123.595	62.306	10.251	1.00	39.82	B	O
ATOM	8487	ND2	ASN	338	121.984	60.845	9.669	1.00	38.06	B	N
ATOM	8488	C	ASN	338	122.216	59.294	13.693	1.00	33.48	B	C
ATOM	8489	O	ASN	338	123.009	59.364	14.631	1.00	33.12	B	O
ATOM	8490	N	CYS	339	121.419	58.251	13.499	1.00	33.60	B	N
ATOM	8491	CA	CYS	339	121.459	57.104	14.385	1.00	34.06	B	C
ATOM	8492	C	CYS	339	121.924	55.913	13.564	1.00	33.56	B	C
ATOM	8493	O	CYS	339	121.135	55.296	12.848	1.00	34.05	B	O
ATOM	8494	CB	CYS	339	120.071	56.829	14.961	1.00	34.96	B	C
ATOM	8495	SG	CYS	339	118.997	58.291	15.160	1.00	37.83	B	S
ATOM	8496	N	LEU	340	123.211	55.604	13.665	1.00	32.80	B	N
ATOM	8497	CA	LEU	340	123.798	54.491	12.933	1.00	33.83	B	C
ATOM	8498	CB	LEU	340	125.303	54.413	13.218	1.00	34.61	B	C
ATOM	8499	CG	LEU	340	126.163	55.530	12.609	1.00	34.61	B	C
ATOM	8500	CD1	LEU	340	127.500	55.633	13.322	1.00	31.70	B	C
ATOM	8501	CD2	LEU	340	126.352	55.257	11.132	1.00	33.80	B	C
ATOM	8502	C	LEU	340	123.152	53.151	13.259	1.00	34.95	B	C
ATOM	8503	O	LEU	340	123.061	52.752	14.418	1.00	34.65	B	O
ATOM	8504	N	VAL	341	122.706	52.457	12.220	1.00	35.87	B	N
ATOM	8505	CA	VAL	341	122.093	51.152	12.387	1.00	36.37	B	C
ATOM	8506	CB	VAL	341	121.981	50.423	11.047	1.00	36.86	B	C
ATOM	8507	CG1	VAL	341	121.012	49.256	11.175	1.00	37.20	B	C
ATOM	8508	CG2	VAL	341	121.532	51.391	9.968	1.00	38.15	B	C
ATOM	8509	C	VAL	341	122.957	50.305	13.314	1.00	36.74	B	C
ATOM	8510	O	VAL	341	122.511	49.872	14.366	1.00	39.77	B	O
ATOM	8511	N	ALA	342	124.200	50.073	12.913	1.00	35.94	B	N
ATOM	8512	CA	ALA	342	125.134	49.283	13.704	1.00	34.75	B	C
ATOM	8513	CB	ALA	342	126.546	49.482	13.178	1.00	34.41	B	C
ATOM	8514	C	ALA	342	125.095	49.609	15.194	1.00	34.74	B	C
ATOM	8515	O	ALA	342	125.698	48.897	16.001	1.00	36.76	B	O
ATOM	8516	N	ARG	343	124.411	50.688	15.561	1.00	32.52	B	N
ATOM	8517	CA	ARG	343	124.303	51.074	16.961	1.00	30.81	B	C
ATOM	8518	CB	ARG	343	124.611	52.562	17.120	1.00	32.62	B	C
ATOM	8519	CG	ARG	343	126.063	52.922	16.844	1.00	34.14	B	C
ATOM	8520	CD	ARG	343	126.345	54.396	17.131	1.00	33.56	B	C
ATOM	8521	NE	ARG	343	127.775	54.692	17.108	1.00	33.70	B	N
ATOM	8522	CZ	ARG	343	128.301	55.885	17.374	1.00	34.14	B	C
ATOM	8523	NH1	ARG	343	127.516	56.907	17.680	1.00	33.88	B	N
ATOM	8524	NH2	ARG	343	129.615	56.052	17.352	1.00	33.78	B	N
ATOM	8525	C	ARG	343	122.919	50.751	17.535	1.00	29.28	B	C

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## FIG. 4 - 175

(Continued)

ATOM	8526	O	ARG	343	122.586	51.143	18.650	1.00	28.30	B	O
ATOM	8527	N	GLN	344	122.121	50.026	16.763	1.00	28.05	B	N
ATOM	8528	CA	GLN	344	120.786	49.625	17.183	1.00	28.26	B	C
ATOM	8529	CB	GLN	344	119.944	49.238	15.974	1.00	26.68	B	C
ATOM	8530	CG	GLN	344	118.980	50.296	15.516	1.00	30.39	B	C
ATOM	8531	CD	GLN	344	118.091	49.802	14.399	1.00	31.50	B	C
ATOM	8532	OE1	GLN	344	117.567	48.685	14.457	1.00	31.52	B	O
ATOM	8533	NE2	GLN	344	117.905	50.632	13.378	1.00	32.84	B	N
ATOM	8534	C	GLN	344	120.853	48.431	18.121	1.00	28.55	B	C
ATOM	8535	O	GLN	344	121.655	47.515	17.919	1.00	28.32	B	O
ATOM	8536	N	HIS	345	120.008	48.436	19.145	1.00	28.34	B	N
ATOM	8537	CA	HIS	345	119.977	47.329	20.085	1.00	28.01	B	C
ATOM	8538	CB	HIS	345	120.514	47.753	21.452	1.00	28.88	B	C
ATOM	8539	CG	HIS	345	121.973	48.079	21.443	1.00	27.88	B	C
ATOM	8540	CD2	HIS	345	123.062	47.279	21.516	1.00	26.67	B	C
ATOM	8541	ND1	HIS	345	122.449	49.361	21.270	1.00	28.37	B	N
ATOM	8542	CE1	HIS	345	123.769	49.337	21.234	1.00	28.14	B	C
ATOM	8543	NE2	HIS	345	124.166	48.086	21.381	1.00	28.63	B	N
ATOM	8544	C	HIS	345	118.568	46.799	20.215	1.00	27.76	B	C
ATOM	8545	O	HIS	345	117.659	47.508	20.625	1.00	30.01	B	O
ATOM	8546	N	ILE	346	118.396	45.538	19.849	1.00	26.83	B	N
ATOM	8547	CA	ILE	346	117.102	44.897	19.899	1.00	25.72	B	C
ATOM	8548	CB	ILE	346	116.977	43.842	18.791	1.00	25.56	B	C
ATOM	8549	CG2	ILE	346	115.655	43.114	18.919	1.00	26.17	B	C
ATOM	8550	CG1	ILE	346	117.102	44.517	17.422	1.00	26.62	B	C
ATOM	8551	CD1	ILE	346	117.180	43.544	16.263	1.00	26.42	B	C
ATOM	8552	C	ILE	346	116.854	44.218	21.228	1.00	26.11	B	C
ATOM	8553	O	ILE	346	117.736	43.558	21.776	1.00	25.75	B	O
ATOM	8554	N	GLU	347	115.645	44.396	21.746	1.00	26.23	B	N
ATOM	8555	CA	GLU	347	115.260	43.767	22.994	1.00	25.82	B	C
ATOM	8556	CB	GLU	347	115.226	44.777	24.134	1.00	25.51	B	C
ATOM	8557	CG	GLU	347	115.282	44.118	25.505	1.00	28.20	B	C
ATOM	8558	CD	GLU	347	115.107	45.094	26.652	1.00	29.16	B	C
ATOM	8559	OE1	GLU	347	115.667	46.208	26.592	1.00	29.18	B	O
ATOM	8560	OE2	GLU	347	114.415	44.736	27.628	1.00	32.76	B	O
ATOM	8561	C	GLU	347	113.873	43.172	22.799	1.00	26.44	B	C
ATOM	8562	O	GLU	347	112.919	43.889	22.495	1.00	26.00	B	O
ATOM	8563	N	MET	348	113.770	41.858	22.957	1.00	26.58	B	N
ATOM	8564	CA	MET	348	112.492	41.181	22.807	1.00	27.90	B	C
ATOM	8565	CB	MET	348	112.270	40.767	21.345	1.00	30.41	B	C
ATOM	8566	CG	MET	348	113.466	40.132	20.660	1.00	34.65	B	C
ATOM	8567	SD	MET	348	113.695	38.420	21.117	1.00	42.21	B	S
ATOM	8568	CE	MET	348	112.733	37.597	19.804	1.00	38.96	B	C
ATOM	8569	C	MET	348	112.371	39.980	23.732	1.00	26.60	B	C
ATOM	8570	O	MET	348	113.363	39.472	24.247	1.00	26.08	B	O
ATOM	8571	N	SER	349	111.135	39.549	23.950	1.00	23.99	B	N
ATOM	8572	CA	SER	349	110.843	38.423	24.812	1.00	21.78	B	C
ATOM	8573	CB	SER	349	109.989	38.894	25.997	1.00	20.79	B	C
ATOM	8574	OG	SER	349	109.402	37.809	26.700	1.00	21.42	B	O

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## FIG. 4 - 176

(Continued)

ATOM	8575	C	SER	349	110.084	37.387	24.005	1.00	21.88	B	C
ATOM	8576	O	SER	349	109.274	37.739	23.154	1.00	23.74	B	O
ATOM	8577	N	THR	350	110.351	36.112	24.264	1.00	21.76	B	N
ATOM	8578	CA	THR	350	109.654	35.033	23.571	1.00	23.08	B	C
ATOM	8579	CB	THR	350	110.603	33.882	23.214	1.00	22.77	B	C
ATOM	8580	OG1	THR	350	111.310	33.483	24.391	1.00	25.37	B	O
ATOM	8581	CG2	THR	350	111.583	34.299	22.152	1.00	22.93	B	C
ATOM	8582	C	THR	350	108.561	34.453	24.475	1.00	22.93	B	C
ATOM	8583	O	THR	350	107.732	33.650	24.035	1.00	20.70	B	O
ATOM	8584	N	THR	351	108.564	34.871	25.737	1.00	22.30	B	N
ATOM	8585	CA	THR	351	107.601	34.366	26.703	1.00	22.35	B	C
ATOM	8586	CB	THR	351	108.332	33.796	27.932	1.00	23.36	B	C
ATOM	8587	OG1	THR	351	108.989	34.859	28.635	1.00	25.67	B	O
ATOM	8588	CG2	THR	351	109.378	32.781	27.493	1.00	22.26	B	C
ATOM	8589	C	THR	351	106.575	35.392	27.171	1.00	21.07	B	C
ATOM	8590	O	THR	351	105.562	35.031	27.760	1.00	20.87	B	O
ATOM	8591	N	GLY	352	106.839	36.668	26.918	1.00	19.83	B	N
ATOM	8592	CA	GLY	352	105.894	37.692	27.325	1.00	19.36	B	C
ATOM	8593	C	GLY	352	106.182	39.027	26.672	1.00	18.63	B	C
ATOM	8594	O	GLY	352	106.633	39.076	25.531	1.00	20.78	B	O
ATOM	8595	N	TRP	353	105.913	40.109	27.397	1.00	17.51	B	N
ATOM	8596	CA	TRP	353	106.156	41.464	26.907	1.00	15.30	B	C
ATOM	8597	CB	TRP	353	105.195	42.451	27.587	1.00	13.08	B	C
ATOM	8598	CG	TRP	353	105.165	42.366	29.084	1.00	9.17	B	C
ATOM	8599	CD2	TRP	353	104.479	41.387	29.877	1.00	7.79	B	C
ATOM	8600	CE2	TRP	353	104.739	41.684	31.233	1.00	8.17	B	C
ATOM	8601	CE3	TRP	353	103.671	40.288	29.574	1.00	10.72	B	C
ATOM	8602	CD1	TRP	353	105.798	43.195	29.966	1.00	11.19	B	C
ATOM	8603	NE1	TRP	353	105.546	42.791	31.265	1.00	10.10	B	N
ATOM	8604	CZ2	TRP	353	104.217	40.921	32.281	1.00	10.66	B	C
ATOM	8605	CZ3	TRP	353	103.149	39.524	30.625	1.00	10.40	B	C
ATOM	8606	CH2	TRP	353	103.426	39.848	31.958	1.00	9.81	B	C
ATOM	8607	C	TRP	353	107.594	41.796	27.264	1.00	15.80	B	C
ATOM	8608	O	TRP	353	108.247	40.999	27.931	1.00	16.59	B	O
ATOM	8609	N	VAL	354	108.092	42.946	26.819	1.00	13.84	B	N
ATOM	8610	CA	VAL	354	109.464	43.338	27.140	1.00	13.65	B	C
ATOM	8611	CB	VAL	354	110.135	44.096	25.960	1.00	16.06	B	C
ATOM	8612	CG1	VAL	354	111.506	44.646	26.400	1.00	12.56	B	C
ATOM	8613	CG2	VAL	354	110.284	43.163	24.751	1.00	12.49	B	C
ATOM	8614	C	VAL	354	109.486	44.248	28.368	1.00	13.83	B	C
ATOM	8615	O	VAL	354	108.716	45.197	28.456	1.00	13.93	B	O
ATOM	8616	N	GLY	355	110.373	43.957	29.313	1.00	14.87	B	N
ATOM	8617	CA	GLY	355	110.467	44.769	30.519	1.00	16.09	B	C
ATOM	8618	C	GLY	355	109.333	44.554	31.513	1.00	16.34	B	C
ATOM	8619	O	GLY	355	108.347	43.877	31.206	1.00	18.25	B	O
ATOM	8620	N	ARG	356	109.456	45.126	32.706	1.00	15.16	B	N
ATOM	8621	CA	ARG	356	108.404	44.953	33.701	1.00	16.32	B	C
ATOM	8622	CB	ARG	356	108.856	45.494	35.066	1.00	14.18	B	C
ATOM	8623	CG	ARG	356	110.001	44.668	35.667	1.00	13.44	B	C

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## FIG. 4 - 177

(Continued)

ATOM	8624	CD	ARG	356	110.169	44.878	37.151	1.00	14.42	B	C
ATOM	8625	NE	ARG	356	111.546	45.211	37.511	1.00	18.65	B	N
ATOM	8626	CZ	ARG	356	112.457	44.341	37.935	1.00	20.17	B	C
ATOM	8627	NH1	ARG	356	112.156	43.055	38.065	1.00	22.71	B	N
ATOM	8628	NH2	ARG	356	113.674	44.765	38.242	1.00	18.93	B	N
ATOM	8629	C	ARG	356	107.111	45.607	33.209	1.00	16.01	B	C
ATOM	8630	O	ARG	356	106.100	44.924	33.066	1.00	16.29	B	O
ATOM	8631	N	PHE	357	107.140	46.911	32.945	1.00	15.89	B	N
ATOM	8632	CA	PHE	357	105.967	47.603	32.402	1.00	16.40	B	C
ATOM	8633	CB	PHE	357	105.418	48.660	33.366	1.00	11.21	B	C
ATOM	8634	CG	PHE	357	104.753	48.083	34.573	1.00	8.48	B	C
ATOM	8635	CD1	PHE	357	105.467	47.878	35.748	1.00	5.58	B	C
ATOM	8636	CD2	PHE	357	103.407	47.711	34.531	1.00	8.57	B	C
ATOM	8637	CE1	PHE	357	104.846	47.309	36.867	1.00	5.98	B	C
ATOM	8638	CE2	PHE	357	102.777	47.136	35.648	1.00	4.59	B	C
ATOM	8639	CZ	PHE	357	103.498	46.937	36.812	1.00	3.60	B	C
ATOM	8640	C	PHE	357	106.344	48.259	31.076	1.00	18.69	B	C
ATOM	8641	O	PHE	357	105.476	48.638	30.287	1.00	21.57	B	O
ATOM	8642	N	ARG	358	107.648	48.377	30.840	1.00	19.12	B	N
ATOM	8643	CA	ARG	358	108.188	48.953	29.612	1.00	19.47	B	C
ATOM	8644	CB	ARG	358	107.826	50.439	29.499	1.00	19.02	B	C
ATOM	8645	CG	ARG	358	108.451	51.346	30.559	1.00	19.99	B	C
ATOM	8646	CD	ARG	358	108.074	52.820	30.338	1.00	22.48	B	C
ATOM	8647	NE	ARG	358	108.633	53.708	31.362	1.00	24.20	B	N
ATOM	8648	CZ	ARG	358	109.204	54.890	31.117	1.00	24.69	B	C
ATOM	8649	NH1	ARG	358	109.304	55.358	29.875	1.00	21.14	B	N
ATOM	8650	NH2	ARG	358	109.696	55.603	32.121	1.00	24.33	B	N
ATOM	8651	C	ARG	358	109.707	48.784	29.646	1.00	20.57	B	C
ATOM	8652	O	ARG	358	110.302	48.704	30.722	1.00	22.16	B	O
ATOM	8653	N	PRO	359	110.355	48.723	28.473	1.00	20.23	B	N
ATOM	8654	CD	PRO	359	109.783	48.894	27.124	1.00	20.61	B	C
ATOM	8655	CA	PRO	359	111.816	48.564	28.411	1.00	20.48	B	C
ATOM	8656	CB	PRO	359	112.137	48.916	26.959	1.00	19.85	B	C
ATOM	8657	CG	PRO	359	110.919	48.431	26.229	1.00	21.21	B	C
ATOM	8658	C	PRO	359	112.527	49.494	29.402	1.00	20.23	B	C
ATOM	8659	O	PRO	359	112.221	50.683	29.465	1.00	22.01	B	O
ATOM	8660	N	SER	360	113.474	48.953	30.163	1.00	19.33	B	N
ATOM	8661	CA	SER	360	114.212	49.725	31.160	1.00	18.75	B	C
ATOM	8662	CB	SER	360	115.122	48.806	31.968	1.00	20.74	B	C
ATOM	8663	OG	SER	360	116.163	48.286	31.149	1.00	26.03	B	O
ATOM	8664	C	SER	360	115.060	50.841	30.560	1.00	18.77	B	C
ATOM	8665	O	SER	360	115.410	50.806	29.382	1.00	17.99	B	O
ATOM	8666	N	GLU	361	115.394	51.824	31.393	1.00	18.96	B	N
ATOM	8667	CA	GLU	361	116.199	52.970	30.978	1.00	18.11	B	C
ATOM	8668	CB	GLU	361	115.982	54.159	31.919	1.00	16.34	B	C
ATOM	8669	CG	GLU	361	116.654	54.007	33.269	1.00	21.67	B	C
ATOM	8670	CD	GLU	361	115.743	53.431	34.342	1.00	27.42	B	C
ATOM	8671	OE1	GLU	361	115.067	52.408	34.091	1.00	28.62	B	O
ATOM	8672	OE2	GLU	361	115.710	54.009	35.453	1.00	31.11	B	O

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(Continued)

## FIG. 4 - 178

ATOM	8673	C	GLU	361	117.674	52.595	31.007	1.00	16.97	B	C
ATOM	8674	O	GLU	361	118.118	51.870	31.888	1.00	16.23	B	O
ATOM	8675	N	PRO	362	118.449	53.079	30.030	1.00	16.09	B	N
ATOM	8676	CD	PRO	362	118.027	53.805	28.817	1.00	13.66	B	C
ATOM	8677	CA	PRO	362	119.879	52.772	29.985	1.00	15.32	B	C
ATOM	8678	CB	PRO	362	120.207	52.916	28.505	1.00	13.19	B	C
ATOM	8679	CG	PRO	362	119.362	54.086	28.121	1.00	12.78	B	C
ATOM	8680	C	PRO	362	120.601	53.806	30.832	1.00	16.34	B	C
ATOM	8681	O	PRO	362	120.096	54.911	31.021	1.00	17.05	B	O
ATOM	8682	N	HIS	363	121.768	53.448	31.353	1.00	17.21	B	N
ATOM	8683	CA	HIS	363	122.550	54.374	32.164	1.00	18.58	B	C
ATOM	8684	CB	HIS	363	122.626	53.875	33.603	1.00	18.05	B	C
ATOM	8685	CG	HIS	363	121.324	53.965	34.333	1.00	19.33	B	C
ATOM	8686	CD2	HIS	363	120.156	53.301	34.158	1.00	19.36	B	C
ATOM	8687	ND1	HIS	363	121.111	54.851	35.368	1.00	18.40	B	N
ATOM	8688	CE1	HIS	363	119.869	54.731	35.799	1.00	19.50	B	C
ATOM	8689	NE2	HIS	363	119.267	53.798	35.081	1.00	22.85	B	N
ATOM	8690	C	HIS	363	123.942	54.499	31.551	1.00	19.40	B	C
ATOM	8691	O	HIS	363	124.833	53.691	31.806	1.00	19.73	B	O
ATOM	8692	N	PHE	364	124.110	55.520	30.723	1.00	19.14	B	N
ATOM	8693	CA	PHE	364	125.371	55.744	30.043	1.00	19.25	B	C
ATOM	8694	CB	PHE	364	125.188	56.802	28.944	1.00	17.71	B	C
ATOM	8695	CG	PHE	364	124.368	56.319	27.777	1.00	15.99	B	C
ATOM	8696	CD1	PHE	364	122.975	56.339	27.826	1.00	12.83	B	C
ATOM	8697	CD2	PHE	364	124.989	55.770	26.656	1.00	12.86	B	C
ATOM	8698	CE1	PHE	364	122.216	55.816	26.781	1.00	8.09	B	C
ATOM	8699	CE2	PHE	364	124.225	55.242	25.607	1.00	10.87	B	C
ATOM	8700	CZ	PHE	364	122.837	55.268	25.679	1.00	7.69	B	C
ATOM	8701	C	PHE	364	126.531	56.127	30.942	1.00	18.72	B	C
ATOM	8702	O	PHE	364	126.341	56.638	32.050	1.00	17.88	B	O
ATOM	8703	N	THR	365	127.735	55.854	30.448	1.00	18.23	B	N
ATOM	8704	CA	THR	365	128.967	56.178	31.159	1.00	19.73	B	C
ATOM	8705	CB	THR	365	130.132	55.288	30.697	1.00	17.73	B	C
ATOM	8706	OG1	THR	365	130.257	55.384	29.275	1.00	22.16	B	O
ATOM	8707	CG2	THR	365	129.890	53.848	31.069	1.00	13.36	B	C
ATOM	8708	C	THR	365	129.312	57.633	30.847	1.00	20.48	B	C
ATOM	8709	O	THR	365	128.662	58.260	30.015	1.00	20.68	B	O
ATOM	8710	N	LEU	366	130.329	58.163	31.515	1.00	22.60	B	N
ATOM	8711	CA	LEU	366	130.740	59.544	31.304	1.00	25.75	B	C
ATOM	8712	CB	LEU	366	132.053	59.831	32.039	1.00	29.32	B	C
ATOM	8713	CG	LEU	366	132.172	59.429	33.516	1.00	34.01	B	C
ATOM	8714	CD1	LEU	366	132.442	57.920	33.631	1.00	33.57	B	C
ATOM	8715	CD2	LEU	366	133.316	60.210	34.162	1.00	34.78	B	C
ATOM	8716	C	LEU	366	130.909	59.900	29.824	1.00	26.20	B	C
ATOM	8717	O	LEU	366	130.317	60.871	29.349	1.00	26.53	B	O
ATOM	8718	N	ASP	367	131.709	59.115	29.102	1.00	24.26	B	N
ATOM	8719	CA	ASP	367	131.964	59.369	27.682	1.00	23.63	B	C
ATOM	8720	CB	ASP	367	133.232	58.636	27.214	1.00	23.47	B	C
ATOM	8721	CG	ASP	367	133.230	57.158	27.582	1.00	25.27	B	C

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(Continued)

## FIG. 4 - 179

ATOM	8722	OD1	ASP	367	132.158	56.515	27.507	1.00	24.35	B	O
ATOM	8723	OD2	ASP	367	134.311	56.634	27.935	1.00	25.99	B	O
ATOM	8724	C	ASP	367	130.810	58.990	26.767	1.00	22.76	B	C
ATOM	8725	O	ASP	367	130.848	59.261	25.568	1.00	24.31	B	O
ATOM	8726	N	GLY	368	129.795	58.348	27.330	1.00	20.91	B	N
ATOM	8727	CA	GLY	368	128.646	57.950	26.547	1.00	18.80	B	C
ATOM	8728	C	GLY	368	128.912	56.843	25.550	1.00	19.81	B	C
ATOM	8729	O	GLY	368	128.059	56.563	24.700	1.00	19.55	B	O
ATOM	8730	N	ASN	369	130.073	56.198	25.643	1.00	19.20	B	N
ATOM	8731	CA	ASN	369	130.398	55.117	24.706	1.00	19.60	B	C
ATOM	8732	CB	ASN	369	131.907	54.986	24.526	1.00	19.65	B	C
ATOM	8733	CG	ASN	369	132.519	56.217	23.921	1.00	21.94	B	C
ATOM	8734	OD1	ASN	369	132.005	56.757	22.945	1.00	25.32	B	O
ATOM	8735	ND2	ASN	369	133.628	56.671	24.489	1.00	23.16	B	N
ATOM	8736	C	ASN	369	129.828	53.760	25.090	1.00	18.53	B	C
ATOM	8737	O	ASN	369	129.770	52.861	24.258	1.00	18.17	B	O
ATOM	8738	N	SER	370	129.420	53.608	26.346	1.00	18.61	B	N
ATOM	8739	CA	SER	370	128.847	52.347	26.812	1.00	19.50	B	C
ATOM	8740	CB	SER	370	129.934	51.447	27.430	1.00	20.45	B	C
ATOM	8741	OG	SER	370	130.577	52.057	28.538	1.00	22.81	B	O
ATOM	8742	C	SER	370	127.746	52.621	27.829	1.00	18.95	B	C
ATOM	8743	O	SER	370	127.562	53.759	28.261	1.00	19.22	B	O
ATOM	8744	N	PHE	371	127.009	51.583	28.209	1.00	18.63	B	N
ATOM	8745	CA	PHE	371	125.931	51.763	29.168	1.00	18.66	B	C
ATOM	8746	CB	PHE	371	124.762	52.516	28.512	1.00	19.79	B	C
ATOM	8747	CG	PHE	371	124.088	51.756	27.398	1.00	16.47	B	C
ATOM	8748	CD1	PHE	371	124.532	51.874	26.093	1.00	15.63	B	C
ATOM	8749	CD2	PHE	371	122.991	50.940	27.660	1.00	17.78	B	C
ATOM	8750	CE1	PHE	371	123.893	51.198	25.059	1.00	18.99	B	C
ATOM	8751	CE2	PHE	371	122.340	50.255	26.631	1.00	18.61	B	C
ATOM	8752	CZ	PHE	371	122.792	50.386	25.327	1.00	18.10	B	C
ATOM	8753	C	PHE	371	125.402	50.473	29.784	1.00	18.78	B	C
ATOM	8754	O	PHE	371	125.506	49.392	29.197	1.00	17.45	B	O
ATOM	8755	N	TYR	372	124.814	50.614	30.970	1.00	19.00	B	N
ATOM	8756	CA	TYR	372	124.240	49.491	31.703	1.00	18.59	B	C
ATOM	8757	CB	TYR	372	124.697	49.527	33.159	1.00	17.86	B	C
ATOM	8758	CG	TYR	372	126.199	49.500	33.290	1.00	17.83	B	C
ATOM	8759	CD1	TYR	372	126.951	50.676	33.201	1.00	19.52	B	C
ATOM	8760	CE1	TYR	372	128.339	50.651	33.257	1.00	18.29	B	C
ATOM	8761	CD2	TYR	372	126.878	48.296	33.441	1.00	17.45	B	C
ATOM	8762	CE2	TYR	372	128.266	48.257	33.498	1.00	18.99	B	C
ATOM	8763	CZ	TYR	372	128.991	49.434	33.405	1.00	18.83	B	C
ATOM	8764	OH	TYR	372	130.364	49.387	33.454	1.00	19.89	B	O
ATOM	8765	C	TYR	372	122.727	49.558	31.620	1.00	18.38	B	C
ATOM	8766	O	TYR	372	122.143	50.632	31.717	1.00	20.19	B	O
ATOM	8767	N	LYS	373	122.096	48.406	31.436	1.00	19.10	B	N
ATOM	8768	CA	LYS	373	120.647	48.340	31.299	1.00	18.51	B	C
ATOM	8769	CB	LYS	373	120.285	48.376	29.809	1.00	17.90	B	C
ATOM	8770	CG	LYS	373	118.809	48.581	29.485	1.00	21.01	B	C

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(Continued)

## FIG. 4 - 180

ATOM	8771	CD	LYS	373	118.593	48.627	27.969	1.00	21.40	B	C
ATOM	8772	CE	LYS	373	117.248	49.238	27.563	1.00	21.67	B	C
ATOM	8773	NZ	LYS	373	116.053	48.389	27.855	1.00	21.98	B	N
ATOM	8774	C	LYS	373	120.128	47.049	31.928	1.00	18.77	B	C
ATOM	8775	O	LYS	373	120.695	45.980	31.712	1.00	18.48	B	O
ATOM	8776	N	ILE	374	119.056	47.150	32.709	1.00	17.06	B	N
ATOM	8777	CA	ILE	374	118.474	45.972	33.332	1.00	15.88	B	C
ATOM	8778	CB	ILE	374	117.557	46.339	34.526	1.00	14.58	B	C
ATOM	8779	CG2	ILE	374	116.955	45.076	35.130	1.00	12.18	B	C
ATOM	8780	CG1	ILE	374	118.348	47.101	35.591	1.00	15.07	B	C
ATOM	8781	CD1	ILE	374	117.517	47.505	36.809	1.00	13.03	B	C
ATOM	8782	C	ILE	374	117.618	45.244	32.303	1.00	16.94	B	C
ATOM	8783	O	ILE	374	116.649	45.803	31.795	1.00	17.41	B	O
ATOM	8784	N	ILE	375	117.977	44.008	31.978	1.00	18.50	B	N
ATOM	8785	CA	ILE	375	117.178	43.226	31.033	1.00	19.71	B	C
ATOM	8786	CB	ILE	375	117.842	43.117	29.625	1.00	19.62	B	C
ATOM	8787	CG2	ILE	375	118.128	44.496	29.070	1.00	19.13	B	C
ATOM	8788	CG1	ILE	375	119.128	42.298	29.706	1.00	21.23	B	C
ATOM	8789	CD1	ILE	375	119.824	42.129	28.373	1.00	23.06	B	C
ATOM	8790	C	ILE	375	116.984	41.815	31.579	1.00	20.44	B	C
ATOM	8791	O	ILE	375	117.735	41.356	32.443	1.00	20.03	B	O
ATOM	8792	N	SER	376	115.968	41.128	31.078	1.00	21.14	B	N
ATOM	8793	CA	SER	376	115.705	39.771	31.516	1.00	21.95	B	C
ATOM	8794	CB	SER	376	114.347	39.318	31.003	1.00	21.55	B	C
ATOM	8795	OG	SER	376	114.026	38.054	31.539	1.00	25.40	B	O
ATOM	8796	C	SER	376	116.808	38.899	30.936	1.00	23.06	B	C
ATOM	8797	O	SER	376	117.236	39.127	29.807	1.00	24.16	B	O
ATOM	8798	N	ASN	377	117.281	37.914	31.698	1.00	24.67	B	N
ATOM	8799	CA	ASN	377	118.358	37.053	31.218	1.00	25.07	B	C
ATOM	8800	CB	ASN	377	119.438	36.891	32.302	1.00	23.49	B	C
ATOM	8801	CG	ASN	377	119.010	35.971	33.444	1.00	23.86	B	C
ATOM	8802	OD1	ASN	377	117.951	35.340	33.397	1.00	23.70	B	O
ATOM	8803	ND2	ASN	377	119.848	35.884	34.474	1.00	20.11	B	N
ATOM	8804	C	ASN	377	117.897	35.681	30.736	1.00	26.79	B	C
ATOM	8805	O	ASN	377	116.706	35.382	30.699	1.00	28.58	B	O
ATOM	8806	N	GLU	378	118.861	34.856	30.353	1.00	29.97	B	N
ATOM	8807	CA	GLU	378	118.608	33.504	29.871	1.00	33.15	B	C
ATOM	8808	CB	GLU	378	119.914	32.716	29.870	1.00	37.08	B	C
ATOM	8809	CG	GLU	378	120.695	32.870	31.181	1.00	43.78	B	C
ATOM	8810	CD	GLU	378	121.681	31.740	31.427	1.00	46.56	B	C
ATOM	8811	OE1	GLU	378	121.225	30.613	31.725	1.00	47.52	B	O
ATOM	8812	OE2	GLU	378	122.906	31.981	31.321	1.00	47.91	B	O
ATOM	8813	C	GLU	378	117.588	32.760	30.722	1.00	33.63	B	C
ATOM	8814	O	GLU	378	116.685	32.113	30.192	1.00	35.16	B	O
ATOM	8815	N	GLU	379	117.740	32.842	32.041	1.00	32.70	B	N
ATOM	8816	CA	GLU	379	116.831	32.160	32.953	1.00	30.44	B	C
ATOM	8817	CB	GLU	379	117.549	31.806	34.256	1.00	34.46	B	C
ATOM	8818	CG	GLU	379	117.845	30.323	34.412	1.00	39.45	B	C
ATOM	8819	CD	GLU	379	116.577	29.475	34.492	1.00	43.32	B	C

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## FIG. 4 - 181

(Continued)

ATOM	8820	OE1	GLU	379	115.800	29.642	35.463	1.00	42.91	B	O
ATOM	8821	OE2	GLU	379	116.357	28.643	33.580	1.00	45.81	B	O
ATOM	8822	C	GLU	379	115.588	32.972	33.265	1.00	28.15	B	C
ATOM	8823	O	GLU	379	114.743	32.539	34.049	1.00	28.12	B	O
ATOM	8824	N	GLY	380	115.473	34.148	32.658	1.00	24.72	B	N
ATOM	8825	CA	GLY	380	114.304	34.980	32.886	1.00	22.38	B	C
ATOM	8826	C	GLY	380	114.335	35.891	34.101	1.00	21.23	B	C
ATOM	8827	O	GLY	380	113.302	36.404	34.514	1.00	21.76	B	O
ATOM	8828	N	TYR	381	115.507	36.084	34.689	1.00	20.24	B	N
ATOM	8829	CA	TYR	381	115.642	36.963	35.842	1.00	19.52	B	C
ATOM	8830	CB	TYR	381	116.539	36.307	36.884	1.00	20.98	B	C
ATOM	8831	CG	TYR	381	115.846	35.194	37.630	1.00	23.80	B	C
ATOM	8832	CD1	TYR	381	115.104	35.465	38.781	1.00	23.87	B	C
ATOM	8833	CE1	TYR	381	114.435	34.458	39.455	1.00	22.94	B	C
ATOM	8834	CD2	TYR	381	115.900	33.876	37.171	1.00	22.81	B	C
ATOM	8835	CE2	TYR	381	115.232	32.859	37.843	1.00	22.55	B	C
ATOM	8836	CZ	TYR	381	114.501	33.161	38.986	1.00	24.14	B	C
ATOM	8837	OH	TYR	381	113.830	32.170	39.667	1.00	25.04	B	O
ATOM	8838	C	TYR	381	116.237	38.292	35.374	1.00	19.14	B	C
ATOM	8839	O	TYR	381	117.178	38.312	34.568	1.00	18.95	B	O
ATOM	8840	N	ARG	382	115.689	39.399	35.871	1.00	15.40	B	N
ATOM	8841	CA	ARG	382	116.160	40.715	35.458	1.00	14.04	B	C
ATOM	8842	CB	ARG	382	115.035	41.738	35.622	1.00	13.48	B	C
ATOM	8843	CG	ARG	382	113.948	41.478	34.606	1.00	15.55	B	C
ATOM	8844	CD	ARG	382	112.581	42.001	34.993	1.00	17.88	B	C
ATOM	8845	NE	ARG	382	111.576	41.337	34.170	1.00	19.19	B	N
ATOM	8846	CZ	ARG	382	111.438	41.515	32.859	1.00	21.25	B	C
ATOM	8847	NH1	ARG	382	112.230	42.357	32.203	1.00	18.86	B	N
ATOM	8848	NH2	ARG	382	110.534	40.810	32.190	1.00	23.20	B	N
ATOM	8849	C	ARG	382	117.438	41.172	36.140	1.00	12.33	B	C
ATOM	8850	O	ARG	382	117.497	41.376	37.349	1.00	9.83	B	O
ATOM	8851	N	HIS	383	118.474	41.303	35.323	1.00	11.97	B	N
ATOM	8852	CA	HIS	383	119.778	41.711	35.789	1.00	12.81	B	C
ATOM	8853	CB	HIS	383	120.714	40.516	35.777	1.00	12.29	B	C
ATOM	8854	CG	HIS	383	120.377	39.496	36.813	1.00	13.83	B	C
ATOM	8855	CD2	HIS	383	119.726	38.313	36.721	1.00	12.69	B	C
ATOM	8856	ND1	HIS	383	120.670	39.675	38.148	1.00	13.84	B	N
ATOM	8857	CE1	HIS	383	120.212	38.643	38.834	1.00	16.23	B	C
ATOM	8858	NE2	HIS	383	119.635	37.803	37.993	1.00	14.04	B	N
ATOM	8859	C	HIS	383	120.351	42.830	34.949	1.00	14.10	B	C
ATOM	8860	O	HIS	383	119.788	43.207	33.913	1.00	15.53	B	O
ATOM	8861	N	ILE	384	121.476	43.354	35.412	1.00	13.75	B	N
ATOM	8862	CA	ILE	384	122.166	44.444	34.749	1.00	15.78	B	C
ATOM	8863	CB	ILE	384	122.996	45.223	35.782	1.00	14.50	B	C
ATOM	8864	CG2	ILE	384	123.765	46.338	35.103	1.00	14.15	B	C
ATOM	8865	CG1	ILE	384	122.071	45.767	36.871	1.00	12.97	B	C
ATOM	8866	CD1	ILE	384	122.791	46.194	38.129	1.00	14.46	B	C
ATOM	8867	C	ILE	384	123.082	43.925	33.645	1.00	18.38	B	C
ATOM	8868	O	ILE	384	123.884	43.014	33.874	1.00	20.02	B	O

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## FIG. 4 - 182

(Continued)

ATOM	8869	N	CYS	385	122.956	44.485	32.446	1.00	19.06	B	N
ATOM	8870	CA	CYS	385	123.812	44.063	31.340	1.00	20.78	B	C
ATOM	8871	C	CYS	385	124.628	45.266	30.868	1.00	19.29	B	C
ATOM	8872	O	CYS	385	124.115	46.376	30.775	1.00	19.30	B	O
ATOM	8873	CB	CYS	385	122.980	43.476	30.178	1.00	22.83	B	C
ATOM	8874	SG	CYS	385	123.868	42.151	29.269	1.00	35.68	B	S
ATOM	8875	N	TYR	386	125.908	45.046	30.595	1.00	18.55	B	N
ATOM	8876	CA	TYR	386	126.795	46.111	30.138	1.00	17.80	B	C
ATOM	8877	CB	TYR	386	128.222	45.849	30.615	1.00	17.85	B	C
ATOM	8878	CG	TYR	386	129.224	46.938	30.295	1.00	17.08	B	C
ATOM	8879	CD1	TYR	386	130.557	46.620	30.049	1.00	18.50	B	C
ATOM	8880	CE1	TYR	386	131.504	47.602	29.797	1.00	20.09	B	C
ATOM	8881	CD2	TYR	386	128.857	48.276	30.279	1.00	17.91	B	C
ATOM	8882	CE2	TYR	386	129.798	49.274	30.032	1.00	21.21	B	C
ATOM	8883	CZ	TYR	386	131.127	48.925	29.791	1.00	21.94	B	C
ATOM	8884	OH	TYR	386	132.082	49.894	29.561	1.00	21.36	B	O
ATOM	8885	C	TYR	386	126.765	46.116	28.625	1.00	17.85	B	C
ATOM	8886	O	TYR	386	126.911	45.069	28.004	1.00	18.61	B	O
ATOM	8887	N	PHE	387	126.573	47.291	28.035	1.00	18.83	B	N
ATOM	8888	CA	PHE	387	126.520	47.418	26.587	1.00	18.83	B	C
ATOM	8889	CB	PHE	387	125.161	47.939	26.133	1.00	17.08	B	C
ATOM	8890	CG	PHE	387	124.014	47.000	26.347	1.00	14.86	B	C
ATOM	8891	CD1	PHE	387	123.409	46.373	25.258	1.00	14.70	B	C
ATOM	8892	CD2	PHE	387	123.444	46.848	27.605	1.00	12.48	B	C
ATOM	8893	CE1	PHE	387	122.246	45.624	25.419	1.00	13.25	B	C
ATOM	8894	CE2	PHE	387	122.283	46.100	27.777	1.00	11.47	B	C
ATOM	8895	CZ	PHE	387	121.680	45.491	26.684	1.00	12.33	B	C
ATOM	8896	C	PHE	387	127.552	48.408	26.057	1.00	21.93	B	C
ATOM	8897	O	PHE	387	127.859	49.413	26.706	1.00	20.79	B	O
ATOM	8898	N	GLN	388	128.057	48.113	24.859	1.00	24.26	B	N
ATOM	8899	CA	GLN	388	128.994	48.970	24.137	1.00	26.10	B	C
ATOM	8900	CB	GLN	388	130.122	48.140	23.534	1.00	26.78	B	C
ATOM	8901	CG	GLN	388	130.905	47.326	24.542	1.00	28.07	B	C
ATOM	8902	CD	GLN	388	131.787	48.185	25.401	1.00	27.71	B	C
ATOM	8903	OE1	GLN	388	132.672	48.871	24.898	1.00	30.29	B	O
ATOM	8904	NE2	GLN	388	131.553	48.160	26.705	1.00	30.63	B	N
ATOM	8905	C	GLN	388	128.074	49.474	23.024	1.00	28.20	B	C
ATOM	8906	O	GLN	388	127.300	48.690	22.478	1.00	28.61	B	O
ATOM	8907	N	ILE	389	128.130	50.755	22.681	1.00	30.33	B	N
ATOM	8908	CA	ILE	389	127.224	51.256	21.650	1.00	32.95	B	C
ATOM	8909	CB	ILE	389	127.233	52.796	21.576	1.00	29.60	B	C
ATOM	8910	CG2	ILE	389	126.839	53.374	22.933	1.00	27.56	B	C
ATOM	8911	CG1	ILE	389	128.606	53.296	21.129	1.00	27.72	B	C
ATOM	8912	CD1	ILE	389	128.699	54.810	21.005	1.00	26.00	B	C
ATOM	8913	C	ILE	389	127.489	50.692	20.261	1.00	37.72	B	C
ATOM	8914	O	ILE	389	126.605	50.705	19.404	1.00	40.02	B	O
ATOM	8915	N	ASP	390	128.696	50.184	20.039	1.00	41.52	B	N
ATOM	8916	CA	ASP	390	129.044	49.621	18.741	1.00	43.97	B	C
ATOM	8917	CB	ASP	390	130.478	50.005	18.365	1.00	45.79	B	C

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## FIG. 4 - 183

(Continued)

ATOM	8918	CG	ASP	390	130.576	51.416	17.816	1.00	49.16	B	C
ATOM	8919	OD1	ASP	390	129.879	51.713	16.819	1.00	50.13	B	O
ATOM	8920	OD2	ASP	390	131.349	52.227	18.372	1.00	50.30	B	O
ATOM	8921	C	ASP	390	128.887	48.106	18.675	1.00	44.93	B	C
ATOM	8922	O	ASP	390	128.589	47.557	17.619	1.00	47.19	B	O
ATOM	8923	N	LYS	391	129.081	47.427	19.798	1.00	45.32	B	N
ATOM	8924	CA	LYS	391	128.967	45.977	19.826	1.00	45.91	B	C
ATOM	8925	CB	LYS	391	129.981	45.409	20.818	1.00	47.86	B	C
ATOM	8926	CG	LYS	391	131.416	45.724	20.407	1.00	51.34	B	C
ATOM	8927	CD	LYS	391	132.428	45.397	21.494	1.00	55.03	B	C
ATOM	8928	CE	LYS	391	133.816	45.911	21.112	1.00	55.62	B	C
ATOM	8929	NZ	LYS	391	134.822	45.719	22.192	1.00	56.68	B	N
ATOM	8930	C	LYS	391	127.550	45.535	20.163	1.00	45.76	B	C
ATOM	8931	O	LYS	391	126.857	46.191	20.942	1.00	46.28	B	O
ATOM	8932	N	LYS	392	127.125	44.419	19.576	1.00	44.97	B	N
ATOM	8933	CA	LYS	392	125.772	43.916	19.782	1.00	45.02	B	C
ATOM	8934	CB	LYS	392	125.218	43.382	18.458	1.00	46.84	B	C
ATOM	8935	CG	LYS	392	124.750	44.494	17.529	1.00	49.00	B	C
ATOM	8936	CD	LYS	392	124.282	43.970	16.186	1.00	50.10	B	C
ATOM	8937	CE	LYS	392	123.533	45.057	15.436	1.00	51.49	B	C
ATOM	8938	NZ	LYS	392	124.298	46.338	15.419	1.00	52.49	B	N
ATOM	8939	C	LYS	392	125.529	42.895	20.886	1.00	43.84	B	C
ATOM	8940	O	LYS	392	124.386	42.512	21.134	1.00	44.15	B	O
ATOM	8941	N	ASP	393	126.579	42.446	21.555	1.00	41.92	B	N
ATOM	8942	CA	ASP	393	126.381	41.489	22.632	1.00	40.21	B	C
ATOM	8943	CB	ASP	393	127.289	40.268	22.470	1.00	41.22	B	C
ATOM	8944	CG	ASP	393	127.022	39.509	21.194	1.00	41.43	B	C
ATOM	8945	OD1	ASP	393	125.838	39.350	20.824	1.00	40.27	B	O
ATOM	8946	OD2	ASP	393	128.005	39.062	20.569	1.00	43.49	B	O
ATOM	8947	C	ASP	393	126.685	42.158	23.953	1.00	38.67	B	C
ATOM	8948	O	ASP	393	127.818	42.588	24.188	1.00	39.07	B	O
ATOM	8949	N	CYS	394	125.678	42.252	24.816	1.00	35.47	B	N
ATOM	8950	CA	CYS	394	125.882	42.870	26.117	1.00	32.02	B	C
ATOM	8951	C	CYS	394	126.374	41.796	27.069	1.00	29.62	B	C
ATOM	8952	O	CYS	394	126.248	40.608	26.787	1.00	29.41	B	O
ATOM	8953	CB	CYS	394	124.586	43.491	26.639	1.00	31.92	B	C
ATOM	8954	SG	CYS	394	123.354	42.328	27.301	1.00	33.67	B	S
ATOM	8955	N	THR	395	126.938	42.215	28.193	1.00	26.53	B	N
ATOM	8956	CA	THR	395	127.462	41.279	29.171	1.00	23.76	B	C
ATOM	8957	CB	THR	395	128.964	41.493	29.358	1.00	23.30	B	C
ATOM	8958	OG1	THR	395	129.627	41.265	28.115	1.00	25.56	B	O
ATOM	8959	CG2	THR	395	129.518	40.542	30.397	1.00	22.48	B	C
ATOM	8960	C	THR	395	126.784	41.448	30.519	1.00	22.20	B	C
ATOM	8961	O	THR	395	126.707	42.556	31.035	1.00	23.25	B	O
ATOM	8962	N	PHE	396	126.300	40.354	31.095	1.00	19.02	B	N
ATOM	8963	CA	PHE	396	125.658	40.444	32.396	1.00	18.94	B	C
ATOM	8964	CB	PHE	396	124.794	39.206	32.652	1.00	17.62	B	C
ATOM	8965	CG	PHE	396	123.486	39.225	31.918	1.00	19.32	B	C
ATOM	8966	CD1	PHE	396	122.477	40.112	32.290	1.00	20.73	B	C

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(Continued)

## FIG. 4 - 184

ATOM	8967	CD2	PHE	396	123.265	38.378	30.837	1.00	19.67	B	C
ATOM	8968	CE1	PHE	396	121.267	40.157	31.593	1.00	21.82	B	C
ATOM	8969	CE2	PHE	396	122.062	38.411	30.130	1.00	20.02	B	C
ATOM	8970	CZ	PHE	396	121.057	39.303	30.507	1.00	22.36	B	C
ATOM	8971	C	PHE	396	126.712	40.596	33.488	1.00	19.09	B	C
ATOM	8972	O	PHE	396	127.703	39.866	33.516	1.00	21.70	B	O
ATOM	8973	N	ILE	397	126.511	41.559	34.380	1.00	17.18	B	N
ATOM	8974	CA	ILE	397	127.454	41.774	35.460	1.00	14.91	B	C
ATOM	8975	CB	ILE	397	127.819	43.240	35.566	1.00	14.47	B	C
ATOM	8976	CG2	ILE	397	128.181	43.762	34.192	1.00	14.09	B	C
ATOM	8977	CG1	ILE	397	126.644	44.036	36.135	1.00	13.14	B	C
ATOM	8978	CD1	ILE	397	126.993	45.472	36.449	1.00	11.32	B	C
ATOM	8979	C	ILE	397	126.885	41.287	36.791	1.00	16.82	B	C
ATOM	8980	O	ILE	397	127.543	41.376	37.833	1.00	18.48	B	O
ATOM	8981	N	THR	398	125.651	40.790	36.753	1.00	15.47	B	N
ATOM	8982	CA	THR	398	125.000	40.241	37.937	1.00	14.86	B	C
ATOM	8983	CB	THR	398	124.049	41.255	38.652	1.00	14.72	B	C
ATOM	8984	OG1	THR	398	122.968	41.627	37.784	1.00	13.55	B	O
ATOM	8985	CG2	THR	398	124.812	42.476	39.083	1.00	13.88	B	C
ATOM	8986	C	THR	398	124.185	39.040	37.490	1.00	15.72	B	C
ATOM	8987	O	THR	398	123.805	38.942	36.323	1.00	15.48	B	O
ATOM	8988	N	LYS	399	123.915	38.127	38.416	1.00	17.12	B	N
ATOM	8989	CA	LYS	399	123.147	36.935	38.094	1.00	18.19	B	C
ATOM	8990	CB	LYS	399	124.026	35.960	37.314	1.00	20.96	B	C
ATOM	8991	CG	LYS	399	125.322	35.630	38.023	1.00	24.93	B	C
ATOM	8992	CD	LYS	399	125.970	34.380	37.458	1.00	29.93	B	C
ATOM	8993	CE	LYS	399	127.055	33.860	38.402	1.00	32.81	B	C
ATOM	8994	NZ	LYS	399	128.082	34.904	38.703	1.00	34.86	B	N
ATOM	8995	C	LYS	399	122.616	36.259	39.354	1.00	17.75	B	C
ATOM	8996	O	LYS	399	123.041	36.571	40.465	1.00	18.35	B	O
ATOM	8997	N	GLY	400	121.684	35.331	39.181	1.00	16.55	B	N
ATOM	8998	CA	GLY	400	121.131	34.640	40.327	1.00	17.62	B	C
ATOM	8999	C	GLY	400	119.616	34.629	40.320	1.00	19.66	B	C
ATOM	9000	O	GLY	400	118.979	35.360	39.551	1.00	22.36	B	O
ATOM	9001	N	THR	401	119.028	33.797	41.172	1.00	18.45	B	N
ATOM	9002	CA	THR	401	117.582	33.708	41.227	1.00	17.93	B	C
ATOM	9003	CB	THR	401	117.125	32.323	41.700	1.00	17.98	B	C
ATOM	9004	OG1	THR	401	117.653	32.056	43.004	1.00	20.05	B	O
ATOM	9005	CG2	THR	401	117.607	31.267	40.730	1.00	13.15	B	C
ATOM	9006	C	THR	401	117.013	34.785	42.125	1.00	16.85	B	C
ATOM	9007	O	THR	401	116.478	34.519	43.192	1.00	18.14	B	O
ATOM	9008	N	TRP	402	117.155	36.013	41.659	1.00	16.42	B	N
ATOM	9009	CA	TRP	402	116.671	37.199	42.335	1.00	14.66	B	C
ATOM	9010	CB	TRP	402	117.528	37.503	43.561	1.00	16.17	B	C
ATOM	9011	CG	TRP	402	119.001	37.502	43.296	1.00	16.85	B	C
ATOM	9012	CD2	TRP	402	119.793	38.614	42.861	1.00	17.78	B	C
ATOM	9013	CE2	TRP	402	121.131	38.164	42.771	1.00	18.27	B	C
ATOM	9014	CE3	TRP	402	119.504	39.948	42.542	1.00	18.13	B	C
ATOM	9015	CD1	TRP	402	119.859	36.453	43.440	1.00	16.20	B	C

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## FIG. 4 - 185

(Continued)

ATOM	9016	NE1	TRP	402	121.143	36.842	43.130	1.00	18.41	B	N
ATOM	9017	CZ2	TRP	402	122.180	39.003	42.378	1.00	16.56	B	C
ATOM	9018	CZ3	TRP	402	120.553	40.784	42.151	1.00	18.56	B	C
ATOM	9019	CH2	TRP	402	121.874	40.303	42.075	1.00	17.33	B	C
ATOM	9020	C	TRP	402	116.827	38.280	41.273	1.00	14.94	B	C
ATOM	9021	O	TRP	402	117.439	38.022	40.229	1.00	14.00	B	O
ATOM	9022	N	GLU	403	116.309	39.480	41.534	1.00	13.41	B	N
ATOM	9023	CA	GLU	403	116.368	40.554	40.548	1.00	12.05	B	C
ATOM	9024	CB	GLU	403	114.990	40.703	39.899	1.00	10.24	B	C
ATOM	9025	CG	GLU	403	114.408	39.396	39.398	1.00	10.20	B	C
ATOM	9026	CD	GLU	403	113.288	39.607	38.391	1.00	14.00	B	C
ATOM	9027	OE1	GLU	403	112.301	40.306	38.713	1.00	15.50	B	O
ATOM	9028	OE2	GLU	403	113.397	39.068	37.271	1.00	14.63	B	O
ATOM	9029	C	GLU	403	116.852	41.938	40.999	1.00	13.29	B	C
ATOM	9030	O	GLU	403	116.785	42.301	42.171	1.00	14.74	B	O
ATOM	9031	N	VAL	404	117.322	42.716	40.031	1.00	12.89	B	N
ATOM	9032	CA	VAL	404	117.800	44.067	40.270	1.00	12.91	B	C
ATOM	9033	CB	VAL	404	118.926	44.420	39.265	1.00	11.91	B	C
ATOM	9034	CG1	VAL	404	119.374	45.859	39.453	1.00	13.92	B	C
ATOM	9035	CG2	VAL	404	120.096	43.484	39.459	1.00	8.31	B	C
ATOM	9036	C	VAL	404	116.607	44.994	40.039	1.00	14.23	B	C
ATOM	9037	O	VAL	404	116.129	45.105	38.918	1.00	16.13	B	O
ATOM	9038	N	ILE	405	116.122	45.653	41.089	1.00	13.56	B	N
ATOM	9039	CA	ILE	405	114.968	46.540	40.951	1.00	12.56	B	C
ATOM	9040	CB	ILE	405	114.453	47.020	42.339	1.00	12.98	B	C
ATOM	9041	CG2	ILE	405	113.151	47.763	42.183	1.00	7.46	B	C
ATOM	9042	CG1	ILE	405	114.256	45.824	43.282	1.00	14.03	B	C
ATOM	9043	CD1	ILE	405	113.390	44.705	42.732	1.00	10.06	B	C
ATOM	9044	C	ILE	405	115.293	47.762	40.088	1.00	14.39	B	C
ATOM	9045	O	ILE	405	114.504	48.156	39.226	1.00	14.58	B	O
ATOM	9046	N	GLY	406	116.455	48.367	40.315	1.00	14.30	B	N
ATOM	9047	CA	GLY	406	116.822	49.521	39.521	1.00	12.80	B	C
ATOM	9048	C	GLY	406	118.253	49.967	39.708	1.00	13.75	B	C
ATOM	9049	O	GLY	406	118.858	49.708	40.737	1.00	16.89	B	O
ATOM	9050	N	ILE	407	118.806	50.618	38.691	1.00	14.84	B	N
ATOM	9051	CA	ILE	407	120.161	51.144	38.760	1.00	13.37	B	C
ATOM	9052	CB	ILE	407	120.797	51.192	37.361	1.00	11.30	B	C
ATOM	9053	CG2	ILE	407	122.039	52.077	37.373	1.00	11.29	B	C
ATOM	9054	CG1	ILE	407	121.163	49.768	36.936	1.00	9.82	B	C
ATOM	9055	CD1	ILE	407	121.237	49.545	35.446	1.00	9.37	B	C
ATOM	9056	C	ILE	407	119.991	52.546	39.343	1.00	15.02	B	C
ATOM	9057	O	ILE	407	119.236	53.361	38.819	1.00	14.39	B	O
ATOM	9058	N	GLU	408	120.692	52.825	40.431	1.00	16.63	B	N
ATOM	9059	CA	GLU	408	120.552	54.105	41.105	1.00	18.23	B	C
ATOM	9060	CB	GLU	408	120.373	53.849	42.601	1.00	21.53	B	C
ATOM	9061	CG	GLU	408	119.290	52.815	42.906	1.00	23.80	B	C
ATOM	9062	CD	GLU	408	117.916	53.275	42.456	1.00	27.87	B	C
ATOM	9063	OE1	GLU	408	117.135	52.429	41.967	1.00	30.29	B	O
ATOM	9064	OE2	GLU	408	117.612	54.483	42.598	1.00	29.06	B	O

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(Continued)

## F I.G. 4 - 1 8 6

ATOM	9065	C	GLU	408	121.687	55.094	40.888	1.00	19.22	B	C
ATOM	9066	O	GLU	408	121.468	56.306	40.924	1.00	21.06	B	O
ATOM	9067	N	ALA	409	122.899	54.589	40.678	1.00	18.36	B	N
ATOM	9068	CA	ALA	409	124.048	55.463	40.473	1.00	17.37	B	C
ATOM	9069	CB	ALA	409	124.533	56.012	41.816	1.00	16.78	B	C
ATOM	9070	C	ALA	409	125.189	54.756	39.755	1.00	17.45	B	C
ATOM	9071	O	ALA	409	125.323	53.536	39.834	1.00	15.91	B	O
ATOM	9072	N	LEU	410	126.009	55.545	39.062	1.00	17.35	B	N
ATOM	9073	CA	LEU	410	127.140	55.034	38.311	1.00	17.53	B	C
ATOM	9074	CB	LEU	410	126.722	54.817	36.857	1.00	16.60	B	C
ATOM	9075	CG	LEU	410	127.767	54.292	35.862	1.00	18.12	B	C
ATOM	9076	CD1	LEU	410	128.278	52.914	36.302	1.00	16.12	B	C
ATOM	9077	CD2	LEU	410	127.144	54.224	34.467	1.00	14.82	B	C
ATOM	9078	C	LEU	410	128.356	55.969	38.356	1.00	18.72	B	C
ATOM	9079	O	LEU	410	128.228	57.175	38.190	1.00	20.28	B	O
ATOM	9080	N	THR	411	129.532	55.396	38.589	1.00	18.37	B	N
ATOM	9081	CA	THR	411	130.786	56.142	38.617	1.00	19.27	B	C
ATOM	9082	CB	THR	411	131.360	56.286	40.060	1.00	18.85	B	C
ATOM	9083	OG1	THR	411	131.869	55.024	40.514	1.00	17.72	B	O
ATOM	9084	CG2	THR	411	130.284	56.764	41.012	1.00	17.11	B	C
ATOM	9085	C	THR	411	131.744	55.293	37.784	1.00	20.67	B	C
ATOM	9086	O	THR	411	131.374	54.200	37.357	1.00	23.60	B	O
ATOM	9087	N	SER	412	132.961	55.772	37.543	1.00	21.07	B	N
ATOM	9088	CA	SER	412	133.912	54.988	36.753	1.00	21.08	B	C
ATOM	9089	CB	SER	412	135.124	55.827	36.365	1.00	18.37	B	C
ATOM	9090	OG	SER	412	135.926	56.086	37.496	1.00	21.11	B	O
ATOM	9091	C	SER	412	134.387	53.778	37.548	1.00	22.07	B	C
ATOM	9092	O	SER	412	134.961	52.843	36.995	1.00	23.13	B	O
ATOM	9093	N	ASP	413	134.144	53.790	38.850	1.00	22.17	B	N
ATOM	9094	CA	ASP	413	134.581	52.677	39.673	1.00	22.98	B	C
ATOM	9095	CB	ASP	413	135.339	53.198	40.895	1.00	25.67	B	C
ATOM	9096	CG	ASP	413	136.731	53.697	40.548	1.00	28.45	B	C
ATOM	9097	OD1	ASP	413	137.338	54.395	41.389	1.00	31.52	B	O
ATOM	9098	OD2	ASP	413	137.228	53.385	39.444	1.00	29.95	B	O
ATOM	9099	C	ASP	413	133.446	51.777	40.123	1.00	22.23	B	C
ATOM	9100	O	ASP	413	133.624	50.565	40.248	1.00	22.67	B	O
ATOM	9101	N	TYR	414	132.274	52.362	40.351	1.00	21.41	B	N
ATOM	9102	CA	TYR	414	131.138	51.575	40.819	1.00	18.45	B	C
ATOM	9103	CB	TYR	414	131.002	51.708	42.329	1.00	15.46	B	C
ATOM	9104	CG	TYR	414	132.101	51.071	43.131	1.00	14.79	B	C
ATOM	9105	CD1	TYR	414	132.118	49.699	43.357	1.00	14.59	B	C
ATOM	9106	CE1	TYR	414	133.093	49.120	44.159	1.00	16.87	B	C
ATOM	9107	CD2	TYR	414	133.093	51.850	43.718	1.00	14.91	B	C
ATOM	9108	CE2	TYR	414	134.071	51.282	44.512	1.00	16.48	B	C
ATOM	9109	CZ	TYR	414	134.066	49.921	44.733	1.00	16.25	B	C
ATOM	9110	OH	TYR	414	135.030	49.369	45.541	1.00	19.68	B	O
ATOM	9111	C	TYR	414	129.787	51.898	40.214	1.00	17.91	B	C
ATOM	9112	O	TYR	414	129.547	52.990	39.693	1.00	17.06	B	O
ATOM	9113	N	LEU	415	128.901	50.917	40.323	1.00	16.46	B	N

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## FIG. 4 - 187

(Continued)

ATOM	9114	CA	LEU	415	127.537	51.027	39.855	1.00	14.70	B	C
ATOM	9115	CB	LEU	415	127.297	50.040	38.714	1.00	13.43	B	C
ATOM	9116	CG	LEU	415	125.924	50.107	38.049	1.00	15.02	B	C
ATOM	9117	CD1	LEU	415	126.044	49.620	36.619	1.00	16.33	B	C
ATOM	9118	CD2	LEU	415	124.899	49.295	38.852	1.00	15.41	B	C
ATOM	9119	C	LEU	415	126.674	50.668	41.066	1.00	15.33	B	C
ATOM	9120	O	LEU	415	126.777	49.566	41.601	1.00	16.82	B	O
ATOM	9121	N	TYR	416	125.840	51.595	41.519	1.00	15.16	B	N
ATOM	9122	CA	TYR	416	124.988	51.313	42.663	1.00	14.80	B	C
ATOM	9123	CB	TYR	416	124.879	52.530	43.566	1.00	13.44	B	C
ATOM	9124	CG	TYR	416	126.201	52.997	44.105	1.00	15.38	B	C
ATOM	9125	CD1	TYR	416	127.031	53.835	43.350	1.00	14.10	B	C
ATOM	9126	CE1	TYR	416	128.240	54.306	43.866	1.00	14.05	B	C
ATOM	9127	CD2	TYR	416	126.618	52.630	45.386	1.00	14.93	B	C
ATOM	9128	CE2	TYR	416	127.823	53.094	45.910	1.00	15.55	B	C
ATOM	9129	CZ	TYR	416	128.625	53.938	45.147	1.00	15.00	B	C
ATOM	9130	OH	TYR	416	129.766	54.466	45.699	1.00	14.00	B	O
ATOM	9131	C	TYR	416	123.604	50.905	42.208	1.00	16.12	B	C
ATOM	9132	O	TYR	416	123.041	51.511	41.296	1.00	16.07	B	O
ATOM	9133	N	TYR	417	123.054	49.878	42.848	1.00	16.79	B	N
ATOM	9134	CA	TYR	417	121.730	49.407	42.482	1.00	18.72	B	C
ATOM	9135	CB	TYR	417	121.840	48.361	41.365	1.00	20.47	B	C
ATOM	9136	CG	TYR	417	122.456	47.039	41.788	1.00	21.65	B	C
ATOM	9137	CD1	TYR	417	121.656	45.983	42.226	1.00	22.60	B	C
ATOM	9138	CE1	TYR	417	122.217	44.760	42.612	1.00	22.32	B	C
ATOM	9139	CD2	TYR	417	123.835	46.843	41.748	1.00	21.40	B	C
ATOM	9140	CE2	TYR	417	124.404	45.626	42.135	1.00	21.84	B	C
ATOM	9141	CZ	TYR	417	123.588	44.590	42.565	1.00	22.22	B	C
ATOM	9142	OH	TYR	417	124.139	43.386	42.950	1.00	22.23	B	O
ATOM	9143	C	TYR	417	120.973	48.824	43.667	1.00	18.97	B	C
ATOM	9144	O	TYR	417	121.523	48.640	44.746	1.00	18.94	B	O
ATOM	9145	N	ILE	418	119.695	48.551	43.453	1.00	19.05	B	N
ATOM	9146	CA	ILE	418	118.857	47.971	44.485	1.00	20.55	B	C
ATOM	9147	CB	ILE	418	117.677	48.906	44.840	1.00	19.77	B	C
ATOM	9148	CG2	ILE	418	116.692	48.187	45.742	1.00	20.86	B	C
ATOM	9149	CG1	ILE	418	118.210	50.148	45.551	1.00	20.46	B	C
ATOM	9150	CD1	ILE	418	117.183	51.211	45.792	1.00	23.81	B	C
ATOM	9151	C	ILE	418	118.337	46.651	43.947	1.00	20.17	B	C
ATOM	9152	O	ILE	418	118.011	46.546	42.767	1.00	21.74	B	O
ATOM	9153	N	SER	419	118.272	45.642	44.808	1.00	19.61	B	N
ATOM	9154	CA	SER	419	117.798	44.327	44.396	1.00	18.91	B	C
ATOM	9155	CB	SER	419	118.969	43.480	43.923	1.00	17.21	B	C
ATOM	9156	OG	SER	419	119.797	43.183	45.030	1.00	19.02	B	O
ATOM	9157	C	SER	419	117.155	43.632	45.578	1.00	18.48	B	C
ATOM	9158	O	SER	419	117.216	44.131	46.699	1.00	19.32	B	O
ATOM	9159	N	ASN	420	116.536	42.481	45.326	1.00	17.64	B	N
ATOM	9160	CA	ASN	420	115.913	41.716	46.395	1.00	16.73	B	C
ATOM	9161	CB	ASN	420	114.448	41.406	46.067	1.00	13.22	B	C
ATOM	9162	CG	ASN	420	114.279	40.740	44.724	1.00	13.67	B	C

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## FIG. 4 - 188

(Continued)

ATOM	9163	OD1	ASN	420	115.220	40.146	44.193	1.00	14.68	B	O
ATOM	9164	ND2	ASN	420	113.072	40.818	44.169	1.00	7.98	B	N
ATOM	9165	C	ASN	420	116.700	40.426	46.638	1.00	16.85	B	C
ATOM	9166	O	ASN	420	116.135	39.368	46.910	1.00	18.37	B	O
ATOM	9167	N	GLU	421	118.018	40.532	46.543	1.00	17.15	B	N
ATOM	9168	CA	GLU	421	118.895	39.393	46.754	1.00	19.34	B	C
ATOM	9169	CB	GLU	421	120.291	39.694	46.195	1.00	18.78	B	C
ATOM	9170	CG	GLU	421	121.358	38.747	46.734	1.00	20.75	B	C
ATOM	9171	CD	GLU	421	122.661	38.782	45.951	1.00	22.48	B	C
ATOM	9172	OE1	GLU	421	123.169	39.890	45.661	1.00	21.18	B	O
ATOM	9173	OE2	GLU	421	123.184	37.689	45.639	1.00	22.04	B	O
ATOM	9174	C	GLU	421	119.028	38.945	48.218	1.00	19.80	B	C
ATOM	9175	O	GLU	421	118.960	37.756	48.519	1.00	20.89	B	O
ATOM	9176	N	TYR	422	119.223	39.897	49.120	1.00	19.38	B	N
ATOM	9177	CA	TYR	422	119.401	39.596	50.530	1.00	19.16	B	C
ATOM	9178	CB	TYR	422	119.386	40.895	51.326	1.00	19.06	B	C
ATOM	9179	CG	TYR	422	119.881	40.746	52.741	1.00	21.59	B	C
ATOM	9180	CD1	TYR	422	121.046	40.023	53.024	1.00	19.84	B	C
ATOM	9181	CE1	TYR	422	121.510	39.893	54.314	1.00	19.73	B	C
ATOM	9182	CD2	TYR	422	119.198	41.334	53.798	1.00	21.32	B	C
ATOM	9183	CE2	TYR	422	119.658	41.210	55.097	1.00	23.82	B	C
ATOM	9184	CZ	TYR	422	120.813	40.488	55.347	1.00	23.64	B	C
ATOM	9185	OH	TYR	422	121.267	40.376	56.637	1.00	28.92	B	O
ATOM	9186	C	TYR	422	118.401	38.600	51.114	1.00	20.84	B	C
ATOM	9187	O	TYR	422	117.187	38.779	51.012	1.00	22.40	B	O
ATOM	9188	N	LYS	423	118.933	37.546	51.732	1.00	21.52	B	N
ATOM	9189	CA	LYS	423	118.130	36.486	52.340	1.00	21.53	B	C
ATOM	9190	CB	LYS	423	117.436	36.995	53.608	1.00	22.83	B	C
ATOM	9191	CG	LYS	423	118.393	37.278	54.751	1.00	25.85	B	C
ATOM	9192	CD	LYS	423	117.677	37.707	56.020	1.00	27.71	B	C
ATOM	9193	CE	LYS	423	118.692	38.082	57.098	1.00	31.46	B	C
ATOM	9194	NZ	LYS	423	118.052	38.548	58.367	1.00	31.96	B	N
ATOM	9195	C	LYS	423	117.097	35.906	51.378	1.00	21.44	B	C
ATOM	9196	O	LYS	423	116.114	35.293	51.797	1.00	22.16	B	O
ATOM	9197	N	GLY	424	117.331	36.106	50.086	1.00	20.50	B	N
ATOM	9198	CA	GLY	424	116.430	35.595	49.070	1.00	20.06	B	C
ATOM	9199	C	GLY	424	114.969	35.945	49.274	1.00	20.45	B	C
ATOM	9200	O	GLY	424	114.102	35.120	49.013	1.00	21.91	B	O
ATOM	9201	N	MET	425	114.695	37.163	49.739	1.00	20.34	B	N
ATOM	9202	CA	MET	425	113.322	37.627	49.968	1.00	18.53	B	C
ATOM	9203	CB	MET	425	113.234	38.329	51.317	1.00	19.68	B	C
ATOM	9204	CG	MET	425	113.756	37.501	52.469	1.00	22.38	B	C
ATOM	9205	SD	MET	425	113.506	38.352	54.020	1.00	24.27	B	S
ATOM	9206	CE	MET	425	111.741	38.663	53.907	1.00	21.26	B	C
ATOM	9207	C	MET	425	112.908	38.604	48.871	1.00	16.75	B	C
ATOM	9208	O	MET	425	113.405	39.725	48.819	1.00	17.33	B	O
ATOM	9209	N	PRO	426	111.968	38.206	47.999	1.00	16.64	B	N
ATOM	9210	CD	PRO	426	111.173	36.969	48.017	1.00	17.29	B	C
ATOM	9211	CA	PRO	426	111.530	39.089	46.910	1.00	15.29	B	C

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## FIG. 4 - 189

(Continued)

ATOM	9212	CB	PRO	426	110.523	38.233	46.140	1.00	15.30	B	C
ATOM	9213	CG	PRO	426	110.816	36.823	46.561	1.00	15.73	B	C
ATOM	9214	C	PRO	426	110.901	40.379	47.416	1.00	15.48	B	C
ATOM	9215	O	PRO	426	110.913	41.402	46.727	1.00	15.90	B	O
ATOM	9216	N	GLY	427	110.362	40.321	48.630	1.00	14.46	B	N
ATOM	9217	CA	GLY	427	109.718	41.480	49.217	1.00	13.34	B	C
ATOM	9218	C	GLY	427	110.649	42.449	49.919	1.00	13.11	B	C
ATOM	9219	O	GLY	427	110.184	43.462	50.452	1.00	14.26	B	O
ATOM	9220	N	GLY	428	111.947	42.144	49.942	1.00	9.68	B	N
ATOM	9221	CA	GLY	428	112.902	43.036	50.577	1.00	8.65	B	C
ATOM	9222	C	GLY	428	113.735	43.771	49.538	1.00	10.35	B	C
ATOM	9223	O	GLY	428	113.778	43.363	48.377	1.00	10.03	B	O
ATOM	9224	N	ARG	429	114.406	44.844	49.946	1.00	11.09	B	N
ATOM	9225	CA	ARG	429	115.224	45.630	49.023	1.00	12.98	B	C
ATOM	9226	CB	ARG	429	114.349	46.667	48.314	1.00	14.68	B	C
ATOM	9227	CG	ARG	429	113.580	46.084	47.144	1.00	18.95	B	C
ATOM	9228	CD	ARG	429	112.423	46.947	46.701	1.00	18.69	B	C
ATOM	9229	NE	ARG	429	111.590	46.279	45.699	1.00	19.88	B	N
ATOM	9230	CZ	ARG	429	111.184	45.008	45.769	1.00	21.09	B	C
ATOM	9231	NH1	ARG	429	111.535	44.227	46.791	1.00	17.36	B	N
ATOM	9232	NH2	ARG	429	110.390	44.520	44.825	1.00	20.65	B	N
ATOM	9233	C	ARG	429	116.420	46.328	49.678	1.00	13.64	B	C
ATOM	9234	O	ARG	429	116.291	46.983	50.707	1.00	13.96	B	O
ATOM	9235	N	ASN	430	117.584	46.198	49.056	1.00	12.81	B	N
ATOM	9236	CA	ASN	430	118.784	46.812	49.585	1.00	13.48	B	C
ATOM	9237	CB	ASN	430	119.605	45.767	50.344	1.00	11.94	B	C
ATOM	9238	CG	ASN	430	118.985	45.411	51.677	1.00	12.47	B	C
ATOM	9239	OD1	ASN	430	119.104	46.167	52.652	1.00	11.56	B	O
ATOM	9240	ND2	ASN	430	118.293	44.277	51.727	1.00	7.39	B	N
ATOM	9241	C	ASN	430	119.644	47.477	48.528	1.00	14.50	B	C
ATOM	9242	O	ASN	430	119.530	47.189	47.335	1.00	14.26	B	O
ATOM	9243	N	LEU	431	120.504	48.377	48.992	1.00	16.18	B	N
ATOM	9244	CA	LEU	431	121.425	49.107	48.135	1.00	17.01	B	C
ATOM	9245	CB	LEU	431	121.709	50.496	48.713	1.00	16.67	B	C
ATOM	9246	CG	LEU	431	122.825	51.279	48.012	1.00	18.10	B	C
ATOM	9247	CD1	LEU	431	122.501	51.399	46.528	1.00	17.30	B	C
ATOM	9248	CD2	LEU	431	122.998	52.651	48.667	1.00	14.93	B	C
ATOM	9249	C	LEU	431	122.729	48.338	48.022	1.00	17.39	B	C
ATOM	9250	O	LEU	431	123.367	48.018	49.028	1.00	19.06	B	O
ATOM	9251	N	TYR	432	123.112	48.038	46.789	1.00	17.62	B	N
ATOM	9252	CA	TYR	432	124.344	47.317	46.511	1.00	18.05	B	C
ATOM	9253	CB	TYR	432	124.061	45.978	45.826	1.00	17.24	B	C
ATOM	9254	CG	TYR	432	123.334	44.944	46.654	1.00	18.80	B	C
ATOM	9255	CD1	TYR	432	121.962	45.034	46.883	1.00	19.62	B	C
ATOM	9256	CE1	TYR	432	121.289	44.049	47.601	1.00	19.23	B	C
ATOM	9257	CD2	TYR	432	124.015	43.843	47.169	1.00	17.63	B	C
ATOM	9258	CE2	TYR	432	123.360	42.862	47.882	1.00	18.49	B	C
ATOM	9259	CZ	TYR	432	121.996	42.968	48.099	1.00	20.13	B	C
ATOM	9260	OH	TYR	432	121.358	41.994	48.834	1.00	21.75	B	O

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## FIG. 4 - 190

(Continued)

ATOM	9261	C	TYR	432	125.193	48.142	45.557	1.00	17.78	B	C
ATOM	9262	O	TYR	432	124.700	49.066	44.903	1.00	18.57	B	O
ATOM	9263	N	LYS	433	126.474	47.805	45.486	1.00	16.13	B	N
ATOM	9264	CA	LYS	433	127.386	48.460	44.563	1.00	14.57	B	C
ATOM	9265	CB	LYS	433	128.237	49.536	45.251	1.00	16.46	B	C
ATOM	9266	CG	LYS	433	129.297	49.022	46.215	1.00	16.27	B	C
ATOM	9267	CD	LYS	433	130.239	50.146	46.606	1.00	16.51	B	C
ATOM	9268	CE	LYS	433	131.190	49.723	47.712	1.00	16.69	B	C
ATOM	9269	NZ	LYS	433	132.101	50.834	48.104	1.00	17.27	B	N
ATOM	9270	C	LYS	433	128.269	47.343	44.058	1.00	13.68	B	C
ATOM	9271	O	LYS	433	128.654	46.454	44.820	1.00	11.44	B	O
ATOM	9272	N	ILE	434	128.564	47.364	42.767	1.00	13.85	B	N
ATOM	9273	CA	ILE	434	129.411	46.331	42.191	1.00	15.56	B	C
ATOM	9274	CB	ILE	434	128.645	45.504	41.124	1.00	14.45	B	C
ATOM	9275	CG2	ILE	434	128.054	46.429	40.061	1.00	11.95	B	C
ATOM	9276	CG1	ILE	434	129.580	44.458	40.518	1.00	14.14	B	C
ATOM	9277	CD1	ILE	434	128.978	43.676	39.379	1.00	14.42	B	C
ATOM	9278	C	ILE	434	130.646	46.973	41.573	1.00	16.13	B	C
ATOM	9279	O	ILE	434	130.554	48.003	40.915	1.00	17.71	B	O
ATOM	9280	N	GLN	435	131.804	46.374	41.809	1.00	18.33	B	N
ATOM	9281	CA	GLN	435	133.045	46.907	41.263	1.00	20.88	B	C
ATOM	9282	CB	GLN	435	134.253	46.264	41.956	1.00	21.76	B	C
ATOM	9283	CG	GLN	435	135.490	47.145	41.958	1.00	24.28	B	C
ATOM	9284	CD	GLN	435	136.715	46.461	42.547	1.00	25.69	B	C
ATOM	9285	OE1	GLN	435	136.763	46.154	43.741	1.00	26.08	B	O
ATOM	9286	NE2	GLN	435	137.713	46.220	41.705	1.00	24.68	B	N
ATOM	9287	C	GLN	435	133.068	46.617	39.767	1.00	20.60	B	C
ATOM	9288	O	GLN	435	132.969	45.465	39.348	1.00	20.57	B	O
ATOM	9289	N	LEU	436	133.200	47.668	38.965	1.00	21.54	B	N
ATOM	9290	CA	LEU	436	133.197	47.527	37.513	1.00	23.39	B	C
ATOM	9291	CB	LEU	436	133.050	48.905	36.880	1.00	21.46	B	C
ATOM	9292	CG	LEU	436	131.785	49.596	37.386	1.00	19.80	B	C
ATOM	9293	CD1	LEU	436	131.748	51.035	36.920	1.00	19.31	B	C
ATOM	9294	CD2	LEU	436	130.572	48.831	36.895	1.00	18.85	B	C
ATOM	9295	C	LEU	436	134.391	46.790	36.908	1.00	25.55	B	C
ATOM	9296	O	LEU	436	134.294	46.242	35.810	1.00	27.46	B	O
ATOM	9297	N	SER	437	135.517	46.775	37.613	1.00	26.98	B	N
ATOM	9298	CA	SER	437	136.690	46.069	37.119	1.00	26.89	B	C
ATOM	9299	CB	SER	437	137.967	46.683	37.689	1.00	26.26	B	C
ATOM	9300	OG	SER	437	137.940	46.694	39.102	1.00	31.19	B	O
ATOM	9301	C	SER	437	136.593	44.597	37.507	1.00	27.29	B	C
ATOM	9302	O	SER	437	137.152	43.736	36.832	1.00	29.17	B	O
ATOM	9303	N	ASP	438	135.882	44.310	38.595	1.00	26.66	B	N
ATOM	9304	CA	ASP	438	135.704	42.930	39.049	1.00	26.32	B	C
ATOM	9305	CB	ASP	438	136.702	42.588	40.151	1.00	28.65	B	C
ATOM	9306	CG	ASP	438	136.622	41.135	40.571	1.00	30.81	B	C
ATOM	9307	OD1	ASP	438	135.517	40.557	40.495	1.00	32.19	B	O
ATOM	9308	OD2	ASP	438	137.659	40.575	40.990	1.00	33.46	B	O
ATOM	9309	C	ASP	438	134.286	42.691	39.572	1.00	24.90	B	C

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(Continued)

## FIG. 4 - 191

ATOM	9310	O	ASP	438	133.959	43.060	40.700	1.00	22.15	B	O
ATOM	9311	N	TYR	439	133.461	42.046	38.753	1.00	23.79	B	N
ATOM	9312	CA	TYR	439	132.083	41.780	39.123	1.00	23.74	B	C
ATOM	9313	CB	TYR	439	131.301	41.243	37.924	1.00	22.94	B	C
ATOM	9314	CG	TYR	439	131.357	42.125	36.698	1.00	22.91	B	C
ATOM	9315	CD1	TYR	439	131.420	43.514	36.814	1.00	22.44	B	C
ATOM	9316	CE1	TYR	439	131.442	44.329	35.687	1.00	22.19	B	C
ATOM	9317	CD2	TYR	439	131.322	41.572	35.416	1.00	22.08	B	C
ATOM	9318	CE2	TYR	439	131.348	42.379	34.285	1.00	21.13	B	C
ATOM	9319	CZ	TYR	439	131.405	43.753	34.430	1.00	21.92	B	C
ATOM	9320	OH	TYR	439	131.410	44.552	33.314	1.00	24.24	B	O
ATOM	9321	C	TYR	439	131.928	40.823	40.294	1.00	24.38	B	C
ATOM	9322	O	TYR	439	130.882	40.801	40.933	1.00	25.27	B	O
ATOM	9323	N	THR	440	132.953	40.030	40.584	1.00	24.21	B	N
ATOM	9324	CA	THR	440	132.858	39.094	41.699	1.00	23.35	B	C
ATOM	9325	CB	THR	440	134.102	38.196	41.806	1.00	23.70	B	C
ATOM	9326	OG1	THR	440	135.221	38.975	42.250	1.00	22.70	B	O
ATOM	9327	CG2	THR	440	134.418	37.568	40.462	1.00	23.82	B	C
ATOM	9328	C	THR	440	132.712	39.852	43.014	1.00	22.79	B	C
ATOM	9329	O	THR	440	132.169	39.328	43.987	1.00	21.81	B	O
ATOM	9330	N	LYS	441	133.200	41.087	43.039	1.00	22.86	B	N
ATOM	9331	CA	LYS	441	133.123	41.905	44.243	1.00	22.90	B	C
ATOM	9332	CB	LYS	441	134.396	42.741	44.375	1.00	25.86	B	C
ATOM	9333	CG	LYS	441	135.620	41.878	44.682	1.00	30.20	B	C
ATOM	9334	CD	LYS	441	136.871	42.702	44.878	1.00	34.36	B	C
ATOM	9335	CE	LYS	441	138.053	41.804	45.201	1.00	37.32	B	C
ATOM	9336	NZ	LYS	441	139.319	42.577	45.346	1.00	40.04	B	N
ATOM	9337	C	LYS	441	131.881	42.794	44.329	1.00	21.89	B	C
ATOM	9338	O	LYS	441	131.828	43.891	43.768	1.00	21.84	B	O
ATOM	9339	N	VAL	442	130.880	42.289	45.039	1.00	19.62	B	N
ATOM	9340	CA	VAL	442	129.624	42.984	45.242	1.00	17.69	B	C
ATOM	9341	CB	VAL	442	128.458	42.093	44.799	1.00	17.33	B	C
ATOM	9342	CG1	VAL	442	127.123	42.770	45.119	1.00	15.79	B	C
ATOM	9343	CG2	VAL	442	128.586	41.792	43.306	1.00	11.20	B	C
ATOM	9344	C	VAL	442	129.502	43.299	46.733	1.00	20.40	B	C
ATOM	9345	O	VAL	442	129.742	42.437	47.572	1.00	22.84	B	O
ATOM	9346	N	THR	443	129.129	44.528	47.066	1.00	20.64	B	N
ATOM	9347	CA	THR	443	129.015	44.927	48.461	1.00	22.17	B	C
ATOM	9348	CB	THR	443	130.040	46.035	48.801	1.00	24.13	B	C
ATOM	9349	OG1	THR	443	131.370	45.566	48.546	1.00	28.90	B	O
ATOM	9350	CG2	THR	443	129.923	46.442	50.255	1.00	22.91	B	C
ATOM	9351	C	THR	443	127.641	45.475	48.819	1.00	23.06	B	C
ATOM	9352	O	THR	443	127.210	46.483	48.254	1.00	26.29	B	O
ATOM	9353	N	CYS	444	126.948	44.835	49.754	1.00	21.88	B	N
ATOM	9354	CA	CYS	444	125.656	45.368	50.163	1.00	22.22	B	C
ATOM	9355	C	CYS	444	125.963	46.516	51.115	1.00	20.79	B	C
ATOM	9356	O	CYS	444	126.866	46.411	51.941	1.00	19.89	B	O
ATOM	9357	CB	CYS	444	124.801	44.328	50.878	1.00	24.50	B	C
ATOM	9358	SG	CYS	444	123.137	44.986	51.221	1.00	27.42	B	S

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## FIG. 4 - 192

(Continued)

ATOM	9359	N	LEU	445	125.205	47.602	51.005	1.00	20.20	B	N
ATOM	9360	CA	LEU	445	125.442	48.785	51.824	1.00	17.71	B	C
ATOM	9361	CB	LEU	445	125.651	49.988	50.899	1.00	15.76	B	C
ATOM	9362	CG	LEU	445	126.714	49.756	49.812	1.00	15.86	B	C
ATOM	9363	CD1	LEU	445	126.930	51.008	48.970	1.00	13.93	B	C
ATOM	9364	CD2	LEU	445	128.007	49.333	50.480	1.00	12.34	B	C
ATOM	9365	C	LEU	445	124.333	49.099	52.814	1.00	19.64	B	C
ATOM	9366	O	LEU	445	124.446	50.036	53.608	1.00	20.41	B	O
ATOM	9367	N	SER	446	123.262	48.314	52.776	1.00	21.11	B	N
ATOM	9368	CA	SER	446	122.131	48.552	53.656	1.00	20.24	B	C
ATOM	9369	CB	SER	446	120.947	49.077	52.834	1.00	20.38	B	C
ATOM	9370	OG	SER	446	120.577	48.143	51.829	1.00	18.25	B	O
ATOM	9371	C	SER	446	121.708	47.307	54.411	1.00	20.86	B	C
ATOM	9372	O	SER	446	121.085	47.404	55.463	1.00	21.91	B	O
ATOM	9373	N	CYS	447	122.043	46.141	53.874	1.00	21.42	B	N
ATOM	9374	CA	CYS	447	121.667	44.875	54.495	1.00	23.05	B	C
ATOM	9375	C	CYS	447	121.845	44.816	56.004	1.00	23.84	B	C
ATOM	9376	O	CYS	447	120.881	44.602	56.739	1.00	24.50	B	O
ATOM	9377	CB	CYS	447	122.461	43.722	53.874	1.00	24.68	B	C
ATOM	9378	SG	CYS	447	122.134	43.458	52.103	1.00	31.64	B	S
ATOM	9379	N	GLU	448	123.080	45.011	56.463	1.00	23.42	B	N
ATOM	9380	CA	GLU	448	123.394	44.913	57.881	1.00	23.49	B	C
ATOM	9381	CB	GLU	448	124.805	44.358	58.061	1.00	24.37	B	C
ATOM	9382	CG	GLU	448	125.060	43.017	57.395	1.00	28.24	B	C
ATOM	9383	CD	GLU	448	123.996	41.985	57.713	1.00	34.11	B	C
ATOM	9384	OE1	GLU	448	123.377	42.073	58.796	1.00	36.48	B	O
ATOM	9385	OE2	GLU	448	123.786	41.070	56.882	1.00	37.27	B	O
ATOM	9386	C	GLU	448	123.249	46.162	58.738	1.00	23.12	B	C
ATOM	9387	O	GLU	448	123.458	46.101	59.948	1.00	24.21	B	O
ATOM	9388	N	LEU	449	122.900	47.289	58.134	1.00	20.81	B	N
ATOM	9389	CA	LEU	449	122.733	48.516	58.899	1.00	20.59	B	C
ATOM	9390	CB	LEU	449	122.123	49.592	58.010	1.00	18.76	B	C
ATOM	9391	CG	LEU	449	123.019	50.143	56.909	1.00	17.31	B	C
ATOM	9392	CD1	LEU	449	122.221	51.089	56.045	1.00	18.95	B	C
ATOM	9393	CD2	LEU	449	124.199	50.868	57.527	1.00	16.25	B	C
ATOM	9394	C	LEU	449	121.853	48.311	60.144	1.00	22.20	B	C
ATOM	9395	O	LEU	449	122.232	48.674	61.261	1.00	22.97	B	O
ATOM	9396	N	ASN	450	120.677	47.731	59.937	1.00	22.75	B	N
ATOM	9397	CA	ASN	450	119.729	47.462	61.011	1.00	21.80	B	C
ATOM	9398	CB	ASN	450	118.958	48.731	61.344	1.00	23.73	B	C
ATOM	9399	CG	ASN	450	118.226	48.632	62.661	1.00	26.67	B	C
ATOM	9400	OD1	ASN	450	117.678	47.581	63.004	1.00	26.78	B	O
ATOM	9401	ND2	ASN	450	118.199	49.733	63.406	1.00	26.73	B	N
ATOM	9402	C	ASN	450	118.772	46.400	60.469	1.00	22.01	B	C
ATOM	9403	O	ASN	450	117.649	46.701	60.072	1.00	21.48	B	O
ATOM	9404	N	PRO	451	119.215	45.134	60.442	1.00	21.65	B	N
ATOM	9405	CD	PRO	451	120.506	44.673	60.969	1.00	20.73	B	C
ATOM	9406	CA	PRO	451	118.430	44.004	59.941	1.00	21.39	B	C
ATOM	9407	CB	PRO	451	119.362	42.817	60.162	1.00	19.94	B	C

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## FIG. 4 - 193

(Continued)

ATOM	9408	CG	PRO	451	120.209	43.253	61.290	1.00	21.78	B	C
ATOM	9409	C	PRO	451	117.035	43.774	60.509	1.00	23.49	B	C
ATOM	9410	O	PRO	451	116.125	43.392	59.774	1.00	25.06	B	O
ATOM	9411	N	GLU	452	116.850	44.003	61.800	1.00	24.25	B	N
ATOM	9412	CA	GLU	452	115.539	43.793	62.394	1.00	26.56	B	C
ATOM	9413	CB	GLU	452	115.650	43.767	63.920	1.00	32.21	B	C
ATOM	9414	CG	GLU	452	116.621	42.720	64.455	1.00	39.54	B	C
ATOM	9415	CD	GLU	452	116.666	42.675	65.976	1.00	44.38	B	C
ATOM	9416	OE1	GLU	452	117.355	41.782	66.521	1.00	47.19	B	O
ATOM	9417	OE2	GLU	452	116.019	43.529	66.627	1.00	46.89	B	O
ATOM	9418	C	GLU	452	114.543	44.867	61.968	1.00	25.59	B	C
ATOM	9419	O	GLU	452	113.374	44.582	61.733	1.00	27.44	B	O
ATOM	9420	N	ARG	453	115.010	46.101	61.848	1.00	23.36	B	N
ATOM	9421	CA	ARG	453	114.132	47.198	61.478	1.00	21.67	B	C
ATOM	9422	CB	ARG	453	114.539	48.463	62.234	1.00	21.94	B	C
ATOM	9423	CG	ARG	453	113.714	49.685	61.872	1.00	20.24	B	C
ATOM	9424	CD	ARG	453	114.165	50.878	62.662	1.00	17.23	B	C
ATOM	9425	NE	ARG	453	113.364	52.058	62.375	1.00	16.99	B	N
ATOM	9426	CZ	ARG	453	113.582	53.245	62.927	1.00	17.21	B	C
ATOM	9427	NH1	ARG	453	114.579	53.391	63.791	1.00	17.27	B	N
ATOM	9428	NH2	ARG	453	112.813	54.280	62.619	1.00	14.66	B	N
ATOM	9429	C	ARG	453	114.077	47.527	59.994	1.00	21.78	B	C
ATOM	9430	O	ARG	453	113.024	47.910	59.477	1.00	20.58	B	O
ATOM	9431	N	CYS	454	115.206	47.368	59.312	1.00	21.64	B	N
ATOM	9432	CA	CYS	454	115.293	47.715	57.903	1.00	19.87	B	C
ATOM	9433	C	CYS	454	115.598	46.616	56.896	1.00	19.70	B	C
ATOM	9434	O	CYS	454	116.698	46.074	56.865	1.00	21.81	B	O
ATOM	9435	CB	CYS	454	116.295	48.847	57.770	1.00	19.47	B	C
ATOM	9436	SG	CYS	454	115.666	50.300	58.650	1.00	18.98	B	S
ATOM	9437	N	GLN	455	114.608	46.332	56.051	1.00	19.11	B	N
ATOM	9438	CA	GLN	455	114.692	45.305	55.015	1.00	14.77	B	C
ATOM	9439	CB	GLN	455	113.881	44.085	55.457	1.00	13.34	B	C
ATOM	9440	CG	GLN	455	114.425	43.413	56.711	1.00	12.92	B	C
ATOM	9441	CD	GLN	455	113.425	42.482	57.387	1.00	13.33	B	C
ATOM	9442	OE1	GLN	455	112.514	41.958	56.749	1.00	14.25	B	O
ATOM	9443	NE2	GLN	455	113.605	42.266	58.688	1.00	13.47	B	N
ATOM	9444	C	GLN	455	114.156	45.815	53.669	1.00	14.10	B	C
ATOM	9445	O	GLN	455	114.058	45.059	52.704	1.00	14.35	B	O
ATOM	9446	N	TYR	456	113.803	47.094	53.597	1.00	13.95	B	N
ATOM	9447	CA	TYR	456	113.268	47.651	52.355	1.00	13.75	B	C
ATOM	9448	CB	TYR	456	111.742	47.600	52.387	1.00	13.55	B	C
ATOM	9449	CG	TYR	456	111.049	47.707	51.045	1.00	10.86	B	C
ATOM	9450	CD1	TYR	456	110.504	46.578	50.436	1.00	10.75	B	C
ATOM	9451	CE1	TYR	456	109.815	46.674	49.236	1.00	9.29	B	C
ATOM	9452	CD2	TYR	456	110.891	48.941	50.405	1.00	9.71	B	C
ATOM	9453	CE2	TYR	456	110.207	49.046	49.200	1.00	4.15	B	C
ATOM	9454	CZ	TYR	456	109.669	47.910	48.629	1.00	8.20	B	C
ATOM	9455	OH	TYR	456	108.949	47.994	47.464	1.00	11.71	B	O
ATOM	9456	C	TYR	456	113.718	49.092	52.190	1.00	14.04	B	C

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(Continued)

## FIG. 4 - 194

ATOM	9457	O	TYR	456	113.127	49.991	52.775	1.00	15.30	B	O
ATOM	9458	N	TYR	457	114.752	49.309	51.382	1.00	15.11	B	N
ATOM	9459	CA	TYR	457	115.286	50.646	51.152	1.00	14.85	B	C
ATOM	9460	CB	TYR	457	116.792	50.674	51.390	1.00	14.57	B	C
ATOM	9461	CG	TYR	457	117.271	50.394	52.786	1.00	14.62	B	C
ATOM	9462	CD1	TYR	457	117.364	49.088	53.275	1.00	14.47	B	C
ATOM	9463	CE1	TYR	457	117.903	48.836	54.540	1.00	14.12	B	C
ATOM	9464	CD2	TYR	457	117.714	51.434	53.595	1.00	13.34	B	C
ATOM	9465	CE2	TYR	457	118.245	51.193	54.850	1.00	13.51	B	C
ATOM	9466	CZ	TYR	457	118.341	49.902	55.318	1.00	11.72	B	C
ATOM	9467	OH	TYR	457	118.877	49.701	56.559	1.00	8.57	B	O
ATOM	9468	C	TYR	457	115.085	51.192	49.742	1.00	15.66	B	C
ATOM	9469	O	TYR	457	114.827	50.455	48.797	1.00	17.46	B	O
ATOM	9470	N	SER	458	115.234	52.505	49.624	1.00	14.42	B	N
ATOM	9471	CA	SER	458	115.176	53.207	48.352	1.00	14.00	B	C
ATOM	9472	CB	SER	458	113.853	53.950	48.163	1.00	12.81	B	C
ATOM	9473	OG	SER	458	113.804	55.138	48.932	1.00	15.84	B	O
ATOM	9474	C	SER	458	116.318	54.175	48.620	1.00	15.10	B	C
ATOM	9475	O	SER	458	116.631	54.431	49.791	1.00	14.29	B	O
ATOM	9476	N	VAL	459	116.946	54.709	47.574	1.00	13.45	B	N
ATOM	9477	CA	VAL	459	118.086	55.593	47.779	1.00	13.00	B	C
ATOM	9478	CB	VAL	459	119.392	54.853	47.433	1.00	13.28	B	C
ATOM	9479	CG1	VAL	459	119.442	54.578	45.934	1.00	10.72	B	C
ATOM	9480	CG2	VAL	459	120.600	55.672	47.878	1.00	13.89	B	C
ATOM	9481	C	VAL	459	118.051	56.882	46.969	1.00	14.23	B	C
ATOM	9482	O	VAL	459	117.283	57.007	46.021	1.00	14.51	B	O
ATOM	9483	N	SER	460	118.901	57.834	47.347	1.00	14.01	B	N
ATOM	9484	CA	SER	460	118.997	59.106	46.643	1.00	14.81	B	C
ATOM	9485	CB	SER	460	118.039	60.116	47.272	1.00	15.45	B	C
ATOM	9486	OG	SER	460	118.038	61.333	46.553	1.00	18.07	B	O
ATOM	9487	C	SER	460	120.442	59.629	46.693	1.00	15.15	B	C
ATOM	9488	O	SER	460	120.930	60.040	47.752	1.00	14.75	B	O
ATOM	9489	N	PHE	461	121.123	59.611	45.547	1.00	14.99	B	N
ATOM	9490	CA	PHE	461	122.516	60.068	45.469	1.00	14.06	B	C
ATOM	9491	CB	PHE	461	123.314	59.229	44.454	1.00	10.57	B	C
ATOM	9492	CG	PHE	461	123.583	57.809	44.885	1.00	8.39	B	C
ATOM	9493	CD1	PHE	461	122.594	56.832	44.792	1.00	7.71	B	C
ATOM	9494	CD2	PHE	461	124.837	57.444	45.367	1.00	6.73	B	C
ATOM	9495	CE1	PHE	461	122.848	55.509	45.172	1.00	6.28	B	C
ATOM	9496	CE2	PHE	461	125.105	56.118	45.752	1.00	6.24	B	C
ATOM	9497	CZ	PHE	461	124.108	55.153	45.653	1.00	6.94	B	C
ATOM	9498	C	PHE	461	122.665	61.533	45.066	1.00	16.79	B	C
ATOM	9499	O	PHE	461	121.833	62.076	44.340	1.00	17.81	B	O
ATOM	9500	N	SER	462	123.740	62.170	45.528	1.00	18.84	B	N
ATOM	9501	CA	SER	462	124.019	63.555	45.155	1.00	20.51	B	C
ATOM	9502	CB	SER	462	125.131	64.137	46.036	1.00	21.92	B	C
ATOM	9503	OG	SER	462	126.346	63.421	45.878	1.00	24.40	B	O
ATOM	9504	C	SER	462	124.465	63.559	43.687	1.00	20.69	B	C
ATOM	9505	O	SER	462	124.607	62.505	43.075	1.00	21.27	B	O

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## FIG. 4 - 195

(Continued)

ATOM	9506	N	LYS	463	124.708	64.736	43.128	1.00	22.99	B	N
ATOM	9507	CA	LYS	463	125.109	64.846	41.728	1.00	25.69	B	C
ATOM	9508	CB	LYS	463	125.483	66.291	41.401	1.00	27.00	B	C
ATOM	9509	CG	LYS	463	124.275	67.189	41.270	1.00	30.44	B	C
ATOM	9510	CD	LYS	463	124.427	68.146	40.097	1.00	35.16	B	C
ATOM	9511	CE	LYS	463	123.083	68.756	39.718	1.00	37.88	B	C
ATOM	9512	NZ	LYS	463	123.169	69.566	38.471	1.00	40.00	B	N
ATOM	9513	C	LYS	463	126.204	63.904	41.230	1.00	26.63	B	C
ATOM	9514	O	LYS	463	126.057	63.297	40.169	1.00	27.72	B	O
ATOM	9515	N	GLU	464	127.305	63.777	41.959	1.00	27.45	B	N
ATOM	9516	CA	GLU	464	128.355	62.868	41.502	1.00	28.40	B	C
ATOM	9517	CB	GLU	464	129.710	63.576	41.429	1.00	31.19	B	C
ATOM	9518	CG	GLU	464	130.079	64.030	40.027	1.00	35.17	B	C
ATOM	9519	CD	GLU	464	129.150	65.100	39.495	1.00	37.56	B	C
ATOM	9520	OE1	GLU	464	129.200	66.229	40.022	1.00	41.38	B	O
ATOM	9521	OE2	GLU	464	128.371	64.817	38.557	1.00	38.51	B	O
ATOM	9522	C	GLU	464	128.476	61.627	42.367	1.00	26.36	B	C
ATOM	9523	O	GLU	464	129.515	60.975	42.379	1.00	25.64	B	O
ATOM	9524	N	ALA	465	127.404	61.302	43.081	1.00	23.96	B	N
ATOM	9525	CA	ALA	465	127.372	60.127	43.936	1.00	21.85	B	C
ATOM	9526	CB	ALA	465	127.663	58.869	43.121	1.00	21.46	B	C
ATOM	9527	C	ALA	465	128.362	60.245	45.074	1.00	20.68	B	C
ATOM	9528	O	ALA	465	128.850	59.244	45.591	1.00	16.26	B	O
ATOM	9529	N	LYS	466	128.661	61.476	45.462	1.00	22.56	B	N
ATOM	9530	CA	LYS	466	129.588	61.693	46.562	1.00	24.73	B	C
ATOM	9531	CB	LYS	466	130.041	63.154	46.609	1.00	25.44	B	C
ATOM	9532	CG	LYS	466	131.173	63.405	47.581	1.00	29.20	B	C
ATOM	9533	CD	LYS	466	131.835	64.762	47.351	1.00	32.39	B	C
ATOM	9534	CE	LYS	466	133.084	64.909	48.218	1.00	34.11	B	C
ATOM	9535	NZ	LYS	466	133.806	66.188	47.965	1.00	36.88	B	N
ATOM	9536	C	LYS	466	128.859	61.318	47.847	1.00	24.27	B	C
ATOM	9537	O	LYS	466	129.469	60.850	48.809	1.00	24.32	B	O
ATOM	9538	N	TYR	467	127.544	61.514	47.846	1.00	22.52	B	N
ATOM	9539	CA	TYR	467	126.722	61.182	49.004	1.00	23.27	B	C
ATOM	9540	CB	TYR	467	126.356	62.441	49.794	1.00	23.00	B	C
ATOM	9541	CG	TYR	467	127.527	63.237	50.292	1.00	24.92	B	C
ATOM	9542	CD1	TYR	467	128.201	64.119	49.451	1.00	25.30	B	C
ATOM	9543	CE1	TYR	467	129.301	64.841	49.902	1.00	26.01	B	C
ATOM	9544	CD2	TYR	467	127.981	63.095	51.604	1.00	26.01	B	C
ATOM	9545	CE2	TYR	467	129.079	63.811	52.064	1.00	26.37	B	C
ATOM	9546	CZ	TYR	467	129.736	64.681	51.206	1.00	26.55	B	C
ATOM	9547	OH	TYR	467	130.841	65.369	51.645	1.00	26.89	B	O
ATOM	9548	C	TYR	467	125.428	60.500	48.584	1.00	22.16	B	C
ATOM	9549	O	TYR	467	125.034	60.557	47.420	1.00	22.32	B	O
ATOM	9550	N	TYR	468	124.775	59.840	49.534	1.00	21.72	B	N
ATOM	9551	CA	TYR	468	123.492	59.208	49.251	1.00	21.47	B	C
ATOM	9552	CB	TYR	468	123.650	57.817	48.614	1.00	19.80	B	C
ATOM	9553	CG	TYR	468	124.468	56.797	49.380	1.00	19.37	B	C
ATOM	9554	CD1	TYR	468	125.844	56.683	49.184	1.00	20.24	B	C

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## FIG. 4 - 196

(Continued)

ATOM	9555	CE1	TYR	468	126.588	55.695	49.833	1.00	20.33	B	C
ATOM	9556	CD2	TYR	468	123.856	55.902	50.252	1.00	19.91	B	C
ATOM	9557	CE2	TYR	468	124.588	54.915	50.909	1.00	19.25	B	C
ATOM	9558	CZ	TYR	468	125.951	54.816	50.695	1.00	20.72	B	C
ATOM	9559	OH	TYR	468	126.674	53.845	51.349	1.00	20.60	B	O
ATOM	9560	C	TYR	468	122.602	59.103	50.474	1.00	21.65	B	C
ATOM	9561	O	TYR	468	123.068	58.836	51.588	1.00	21.59	B	O
ATOM	9562	N	GLN	469	121.317	59.360	50.268	1.00	19.96	B	N
ATOM	9563	CA	GLN	469	120.369	59.235	51.355	1.00	18.78	B	C
ATOM	9564	CB	GLN	469	119.277	60.302	51.283	1.00	16.79	B	C
ATOM	9565	CG	GLN	469	118.247	60.143	52.393	1.00	16.33	B	C
ATOM	9566	CD	GLN	469	117.035	61.034	52.214	1.00	16.44	B	C
ATOM	9567	OE1	GLN	469	116.438	61.076	51.147	1.00	18.52	B	O
ATOM	9568	NE2	GLN	469	116.659	61.739	53.265	1.00	16.60	B	N
ATOM	9569	C	GLN	469	119.729	57.855	51.240	1.00	18.75	B	C
ATOM	9570	O	GLN	469	119.353	57.413	50.156	1.00	20.25	B	O
ATOM	9571	N	LEU	470	119.641	57.160	52.359	1.00	18.03	B	N
ATOM	9572	CA	LEU	470	119.013	55.862	52.383	1.00	16.05	B	C
ATOM	9573	CB	LEU	470	119.871	54.860	53.153	1.00	12.88	B	C
ATOM	9574	CG	LEU	470	120.920	54.116	52.334	1.00	7.18	B	C
ATOM	9575	CD1	LEU	470	121.669	53.176	53.230	1.00	9.83	B	C
ATOM	9576	CD2	LEU	470	120.248	53.344	51.241	1.00	5.95	B	C
ATOM	9577	C	LEU	470	117.674	56.055	53.077	1.00	18.52	B	C
ATOM	9578	O	LEU	470	117.573	56.769	54.082	1.00	17.50	B	O
ATOM	9579	N	ARG	471	116.644	55.437	52.517	1.00	20.97	B	N
ATOM	9580	CA	ARG	471	115.306	55.521	53.070	1.00	23.15	B	C
ATOM	9581	CB	ARG	471	114.354	56.203	52.085	1.00	25.88	B	C
ATOM	9582	CG	ARG	471	112.907	56.240	52.553	1.00	31.75	B	C
ATOM	9583	CD	ARG	471	111.997	56.927	51.541	1.00	35.75	B	C
ATOM	9584	NE	ARG	471	110.677	57.213	52.102	1.00	39.62	B	N
ATOM	9585	CZ	ARG	471	109.737	57.920	51.478	1.00	41.33	B	C
ATOM	9586	NH1	ARG	471	109.972	58.412	50.269	1.00	41.52	B	N
ATOM	9587	NH2	ARG	471	108.564	58.142	52.063	1.00	40.93	B	N
ATOM	9588	C	ARG	471	114.826	54.112	53.345	1.00	24.13	B	C
ATOM	9589	O	ARG	471	114.604	53.323	52.425	1.00	25.84	B	O
ATOM	9590	N	CYS	472	114.687	53.796	54.621	1.00	23.64	B	N
ATOM	9591	CA	CYS	472	114.219	52.487	55.042	1.00	23.00	B	C
ATOM	9592	C	CYS	472	112.732	52.636	55.321	1.00	21.14	B	C
ATOM	9593	O	CYS	472	112.323	53.547	56.036	1.00	21.12	B	O
ATOM	9594	CB	CYS	472	114.981	52.073	56.299	1.00	23.91	B	C
ATOM	9595	SG	CYS	472	114.149	50.907	57.416	1.00	27.85	B	S
ATOM	9596	N	SER	473	111.919	51.755	54.756	1.00	19.44	B	N
ATOM	9597	CA	SER	473	110.482	51.846	54.967	1.00	18.92	B	C
ATOM	9598	CB	SER	473	109.789	52.191	53.646	1.00	18.36	B	C
ATOM	9599	OG	SER	473	110.141	51.261	52.642	1.00	21.93	B	O
ATOM	9600	C	SER	473	109.832	50.609	55.581	1.00	17.21	B	C
ATOM	9601	O	SER	473	108.615	50.465	55.530	1.00	19.59	B	O
ATOM	9602	N	GLY	474	110.629	49.716	56.156	1.00	16.48	B	N
ATOM	9603	CA	GLY	474	110.055	48.532	56.771	1.00	16.90	B	C

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## FIG. 4 - 197

(Continued)

ATOM	9604	C	GLY	474	111.040	47.425	57.091	1.00	16.48	B	C
ATOM	9605	O	GLY	474	112.149	47.403	56.563	1.00	18.05	B	O
ATOM	9606	N	PRO	475	110.643	46.446	57.913	1.00	16.25	B	N
ATOM	9607	CD	PRO	475	111.562	45.333	58.219	1.00	17.27	B	C
ATOM	9608	CA	PRO	475	109.353	46.249	58.584	1.00	14.24	B	C
ATOM	9609	CB	PRO	475	109.445	44.807	59.068	1.00	13.06	B	C
ATOM	9610	CG	PRO	475	110.896	44.680	59.411	1.00	14.77	B	C
ATOM	9611	C	PRO	475	109.012	47.214	59.716	1.00	14.52	B	C
ATOM	9612	O	PRO	475	107.840	47.392	60.041	1.00	16.67	B	O
ATOM	9613	N	GLY	476	110.023	47.818	60.331	1.00	14.14	B	N
ATOM	9614	CA	GLY	476	109.770	48.750	61.415	1.00	11.62	B	C
ATOM	9615	C	GLY	476	109.524	50.140	60.868	1.00	12.63	B	C
ATOM	9616	O	GLY	476	109.407	50.307	59.656	1.00	12.58	B	O
ATOM	9617	N	LEU	477	109.454	51.137	61.748	1.00	11.74	B	N
ATOM	9618	CA	LEU	477	109.222	52.519	61.331	1.00	11.92	B	C
ATOM	9619	CB	LEU	477	109.072	53.412	62.563	1.00	10.87	B	C
ATOM	9620	CG	LEU	477	107.928	53.053	63.514	1.00	13.02	B	C
ATOM	9621	CD1	LEU	477	107.940	54.009	64.698	1.00	12.46	B	C
ATOM	9622	CD2	LEU	477	106.586	53.114	62.775	1.00	12.47	B	C
ATOM	9623	C	LEU	477	110.325	53.086	60.414	1.00	13.40	B	C
ATOM	9624	O	LEU	477	111.516	52.819	60.604	1.00	11.34	B	O
ATOM	9625	N	PRO	478	109.931	53.894	59.414	1.00	13.58	B	N
ATOM	9626	CD	PRO	478	108.541	54.283	59.121	1.00	14.52	B	C
ATOM	9627	CA	PRO	478	110.852	54.510	58.455	1.00	14.07	B	C
ATOM	9628	CB	PRO	478	109.962	55.495	57.705	1.00	13.81	B	C
ATOM	9629	CG	PRO	478	108.638	54.795	57.702	1.00	14.19	B	C
ATOM	9630	C	PRO	478	112.033	55.188	59.118	1.00	15.11	B	C
ATOM	9631	O	PRO	478	111.892	55.820	60.163	1.00	16.31	B	O
ATOM	9632	N	LEU	479	113.197	55.048	58.490	1.00	16.04	B	N
ATOM	9633	CA	LEU	479	114.444	55.621	58.982	1.00	15.01	B	C
ATOM	9634	CB	LEU	479	115.279	54.528	59.657	1.00	13.83	B	C
ATOM	9635	CG	LEU	479	116.675	54.866	60.179	1.00	12.46	B	C
ATOM	9636	CD1	LEU	479	116.606	55.990	61.189	1.00	13.23	B	C
ATOM	9637	CD2	LEU	479	117.268	53.631	60.813	1.00	12.22	B	C
ATOM	9638	C	LEU	479	115.204	56.217	57.801	1.00	14.97	B	C
ATOM	9639	O	LEU	479	115.395	55.557	56.783	1.00	15.80	B	O
ATOM	9640	N	TYR	480	115.627	57.468	57.940	1.00	15.76	B	N
ATOM	9641	CA	TYR	480	116.350	58.165	56.883	1.00	16.51	B	C
ATOM	9642	CB	TYR	480	115.631	59.471	56.517	1.00	18.80	B	C
ATOM	9643	CG	TYR	480	114.210	59.293	56.024	1.00	20.33	B	C
ATOM	9644	CD1	TYR	480	113.910	59.364	54.664	1.00	22.57	B	C
ATOM	9645	CE1	TYR	480	112.604	59.161	54.196	1.00	23.68	B	C
ATOM	9646	CD2	TYR	480	113.170	59.019	56.915	1.00	20.23	B	C
ATOM	9647	CE2	TYR	480	111.870	58.815	56.464	1.00	22.45	B	C
ATOM	9648	CZ	TYR	480	111.591	58.885	55.102	1.00	24.15	B	C
ATOM	9649	OH	TYR	480	110.312	58.658	54.648	1.00	24.41	B	O
ATOM	9650	C	TYR	480	117.744	58.483	57.379	1.00	15.96	B	C
ATOM	9651	O	TYR	480	117.910	59.005	58.482	1.00	15.89	B	O
ATOM	9652	N	THR	481	118.743	58.179	56.559	1.00	15.76	B	N

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(Continued)

## FIG. 4 - 198

ATOM	9653	CA	THR	481	120.129	58.431	56.924	1.00	15.65	B	C
ATOM	9654	CB	THR	481	120.774	57.163	57.480	1.00	14.54	B	C
ATOM	9655	OG1	THR	481	120.459	56.065	56.622	1.00	18.10	B	O
ATOM	9656	CG2	THR	481	120.256	56.864	58.858	1.00	15.87	B	C
ATOM	9657	C	THR	481	120.964	58.919	55.752	1.00	16.24	B	C
ATOM	9658	O	THR	481	120.650	58.648	54.602	1.00	16.93	B	O
ATOM	9659	N	LEU	482	122.035	59.646	56.058	1.00	18.90	B	N
ATOM	9660	CA	LEU	482	122.937	60.166	55.038	1.00	19.21	B	C
ATOM	9661	CB	LEU	482	123.203	61.653	55.279	1.00	20.10	B	C
ATOM	9662	CG	LEU	482	123.765	62.439	54.092	1.00	21.90	B	C
ATOM	9663	CD1	LEU	482	122.736	62.475	52.975	1.00	21.10	B	C
ATOM	9664	CD2	LEU	482	124.115	63.856	54.525	1.00	22.66	B	C
ATOM	9665	C	LEU	482	124.243	59.373	55.121	1.00	19.39	B	C
ATOM	9666	O	LEU	482	124.684	59.013	56.210	1.00	20.79	B	O
ATOM	9667	N	HIS	483	124.849	59.096	53.970	1.00	18.33	B	N
ATOM	9668	CA	HIS	483	126.090	58.332	53.903	1.00	16.79	B	C
ATOM	9669	CB	HIS	483	125.791	56.894	53.488	1.00	14.55	B	C
ATOM	9670	CG	HIS	483	124.697	56.245	54.276	1.00	14.89	B	C
ATOM	9671	CD2	HIS	483	123.358	56.434	54.264	1.00	15.13	B	C
ATOM	9672	ND1	HIS	483	124.933	55.258	55.211	1.00	16.09	B	N
ATOM	9673	CE1	HIS	483	123.788	54.867	55.736	1.00	13.84	B	C
ATOM	9674	NE2	HIS	483	122.816	55.565	55.178	1.00	14.31	B	N
ATOM	9675	C	HIS	483	127.043	58.939	52.868	1.00	18.94	B	C
ATOM	9676	O	HIS	483	126.617	59.665	51.961	1.00	19.56	B	O
ATOM	9677	N	SER	484	128.333	58.645	53.003	1.00	19.52	B	N
ATOM	9678	CA	SER	484	129.318	59.131	52.040	1.00	21.33	B	C
ATOM	9679	CB	SER	484	130.520	59.779	52.738	1.00	21.77	B	C
ATOM	9680	OG	SER	484	131.351	58.803	53.344	1.00	24.25	B	O
ATOM	9681	C	SER	484	129.774	57.907	51.259	1.00	21.22	B	C
ATOM	9682	O	SER	484	129.942	56.827	51.830	1.00	19.26	B	O
ATOM	9683	N	SER	485	129.979	58.076	49.960	1.00	22.12	B	N
ATOM	9684	CA	SER	485	130.389	56.967	49.110	1.00	25.62	B	C
ATOM	9685	CB	SER	485	130.095	57.301	47.645	1.00	26.28	B	C
ATOM	9686	OG	SER	485	128.715	57.552	47.444	1.00	30.40	B	O
ATOM	9687	C	SER	485	131.840	56.495	49.221	1.00	26.33	B	C
ATOM	9688	O	SER	485	132.097	55.300	49.138	1.00	27.23	B	O
ATOM	9689	N	VAL	486	132.781	57.416	49.407	1.00	28.07	B	N
ATOM	9690	CA	VAL	486	134.194	57.056	49.468	1.00	29.41	B	C
ATOM	9691	CB	VAL	486	135.084	58.284	49.798	1.00	30.37	B	C
ATOM	9692	CG1	VAL	486	134.786	58.797	51.192	1.00	31.49	B	C
ATOM	9693	CG2	VAL	486	136.553	57.909	49.665	1.00	30.81	B	C
ATOM	9694	C	VAL	486	134.507	55.929	50.442	1.00	30.57	B	C
ATOM	9695	O	VAL	486	135.269	55.016	50.119	1.00	31.62	B	O
ATOM	9696	N	ASN	487	133.922	55.979	51.630	1.00	30.95	B	N
ATOM	9697	CA	ASN	487	134.159	54.928	52.610	1.00	31.75	B	C
ATOM	9698	CB	ASN	487	134.888	55.498	53.833	1.00	35.87	B	C
ATOM	9699	CG	ASN	487	136.336	55.868	53.537	1.00	38.55	B	C
ATOM	9700	OD1	ASN	487	136.838	56.895	54.014	1.00	38.47	B	O
ATOM	9701	ND2	ASN	487	137.019	55.026	52.759	1.00	37.49	B	N

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## FIG. 4 - 199

(Continued)

ATOM	9702	C	ASN	487	132.850	54.288	53.048	1.00	30.74	B	C
ATOM	9703	O	ASN	487	132.830	53.486	53.982	1.00	31.45	B	O
ATOM	9704	N	ASP	488	131.762	54.633	52.364	1.00	28.68	B	N
ATOM	9705	CA	ASP	488	130.449	54.108	52.707	1.00	26.66	B	C
ATOM	9706	CB	ASP	488	130.331	52.636	52.313	1.00	27.90	B	C
ATOM	9707	CG	ASP	488	130.253	52.440	50.816	1.00	29.72	B	C
ATOM	9708	OD1	ASP	488	129.461	53.146	50.161	1.00	31.30	B	O
ATOM	9709	OD2	ASP	488	130.977	51.572	50.290	1.00	32.18	B	O
ATOM	9710	C	ASP	488	130.219	54.259	54.204	1.00	25.72	B	C
ATOM	9711	O	ASP	488	129.654	53.382	54.856	1.00	24.30	B	O
ATOM	9712	N	LYS	489	130.669	55.378	54.754	1.00	25.25	B	N
ATOM	9713	CA	LYS	489	130.503	55.610	56.176	1.00	24.10	B	C
ATOM	9714	CB	LYS	489	131.607	56.529	56.705	1.00	24.94	B	C
ATOM	9715	CG	LYS	489	131.622	57.898	56.069	1.00	29.19	B	C
ATOM	9716	CD	LYS	489	132.805	58.719	56.560	1.00	33.11	B	C
ATOM	9717	CE	LYS	489	132.771	60.133	55.995	1.00	34.94	B	C
ATOM	9718	NZ	LYS	489	133.883	60.959	56.541	1.00	39.70	B	N
ATOM	9719	C	LYS	489	129.140	56.216	56.449	1.00	22.29	B	C
ATOM	9720	O	LYS	489	128.556	56.872	55.585	1.00	20.15	B	O
ATOM	9721	N	GLY	490	128.639	55.968	57.657	1.00	22.04	B	N
ATOM	9722	CA	GLY	490	127.352	56.487	58.067	1.00	20.03	B	C
ATOM	9723	C	GLY	490	127.545	57.854	58.676	1.00	20.18	B	C
ATOM	9724	O	GLY	490	128.091	57.989	59.769	1.00	20.54	B	O
ATOM	9725	N	LEU	491	127.092	58.876	57.965	1.00	19.44	B	N
ATOM	9726	CA	LEU	491	127.234	60.233	58.440	1.00	19.54	B	C
ATOM	9727	CB	LEU	491	127.032	61.203	57.283	1.00	20.53	B	C
ATOM	9728	CG	LEU	491	128.153	61.167	56.242	1.00	18.39	B	C
ATOM	9729	CD1	LEU	491	127.831	62.089	55.090	1.00	19.23	B	C
ATOM	9730	CD2	LEU	491	129.441	61.577	56.898	1.00	18.31	B	C
ATOM	9731	C	LEU	491	126.287	60.555	59.586	1.00	20.91	B	C
ATOM	9732	O	LEU	491	126.735	60.780	60.713	1.00	22.15	B	O
ATOM	9733	N	ARG	492	124.984	60.566	59.316	1.00	20.73	B	N
ATOM	9734	CA	ARG	492	124.020	60.881	60.364	1.00	20.06	B	C
ATOM	9735	CB	ARG	492	124.036	62.382	60.644	1.00	20.71	B	C
ATOM	9736	CG	ARG	492	123.393	63.244	59.568	1.00	20.08	B	C
ATOM	9737	CD	ARG	492	123.759	64.698	59.798	1.00	21.15	B	C
ATOM	9738	NE	ARG	492	125.193	64.888	59.625	1.00	21.60	B	N
ATOM	9739	CZ	ARG	492	125.765	65.192	58.466	1.00	23.12	B	C
ATOM	9740	NH1	ARG	492	125.022	65.360	57.380	1.00	24.47	B	N
ATOM	9741	NH2	ARG	492	127.083	65.286	58.383	1.00	23.72	B	N
ATOM	9742	C	ARG	492	122.585	60.443	60.085	1.00	21.47	B	C
ATOM	9743	O	ARG	492	122.247	59.998	58.983	1.00	21.32	B	O
ATOM	9744	N	VAL	493	121.746	60.580	61.107	1.00	20.97	B	N
ATOM	9745	CA	VAL	493	120.344	60.211	61.018	1.00	21.38	B	C
ATOM	9746	CB	VAL	493	119.883	59.537	62.325	1.00	22.41	B	C
ATOM	9747	CG1	VAL	493	118.402	59.215	62.247	1.00	23.17	B	C
ATOM	9748	CG2	VAL	493	120.698	58.266	62.574	1.00	20.83	B	C
ATOM	9749	C	VAL	493	119.497	61.456	60.763	1.00	21.55	B	C
ATOM	9750	O	VAL	493	119.462	62.371	61.580	1.00	21.85	B	O

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## FIG. 4 - 200

(Continued)

ATOM	9751	N	LEU	494	118.811	61.485	59.626	1.00	21.18	B	N
ATOM	9752	CA	LEU	494	117.974	62.626	59.264	1.00	19.43	B	C
ATOM	9753	CB	LEU	494	117.782	62.660	57.742	1.00	19.57	B	C
ATOM	9754	CG	LEU	494	119.101	62.610	56.953	1.00	21.60	B	C
ATOM	9755	CD1	LEU	494	118.832	62.502	55.456	1.00	20.38	B	C
ATOM	9756	CD2	LEU	494	119.929	63.851	57.271	1.00	19.91	B	C
ATOM	9757	C	LEU	494	116.615	62.576	59.964	1.00	18.58	B	C
ATOM	9758	O	LEU	494	116.111	63.595	60.443	1.00	18.81	B	O
ATOM	9759	N	GLU	495	116.025	61.390	60.022	1.00	16.24	B	N
ATOM	9760	CA	GLU	495	114.729	61.225	60.659	1.00	16.44	B	C
ATOM	9761	CB	GLU	495	113.612	61.651	59.698	1.00	17.53	B	C
ATOM	9762	CG	GLU	495	112.217	61.506	60.268	1.00	19.67	B	C
ATOM	9763	CD	GLU	495	111.984	62.399	61.476	1.00	22.97	B	C
ATOM	9764	OE1	GLU	495	112.023	63.642	61.315	1.00	22.51	B	O
ATOM	9765	OE2	GLU	495	111.767	61.858	62.585	1.00	22.70	B	O
ATOM	9766	C	GLU	495	114.553	59.770	61.059	1.00	14.79	B	C
ATOM	9767	O	GLU	495	114.678	58.875	60.236	1.00	15.37	B	O
ATOM	9768	N	ASP	496	114.264	59.534	62.329	1.00	14.29	B	N
ATOM	9769	CA	ASP	496	114.100	58.175	62.811	1.00	13.80	B	C
ATOM	9770	CB	ASP	496	115.128	57.867	63.909	1.00	14.57	B	C
ATOM	9771	CG	ASP	496	114.938	58.715	65.154	1.00	12.87	B	C
ATOM	9772	OD1	ASP	496	113.849	59.297	65.330	1.00	12.34	B	O
ATOM	9773	OD2	ASP	496	115.882	58.789	65.971	1.00	13.20	B	O
ATOM	9774	C	ASP	496	112.711	57.895	63.341	1.00	13.42	B	C
ATOM	9775	O	ASP	496	112.453	56.808	63.845	1.00	14.36	B	O
ATOM	9776	N	ASN	497	111.820	58.871	63.234	1.00	12.87	B	N
ATOM	9777	CA	ASN	497	110.460	58.697	63.717	1.00	15.91	B	C
ATOM	9778	CB	ASN	497	109.736	57.666	62.855	1.00	16.28	B	C
ATOM	9779	CG	ASN	497	109.227	58.255	61.564	1.00	20.09	B	C
ATOM	9780	OD1	ASN	497	108.308	59.077	61.570	1.00	18.95	B	O
ATOM	9781	ND2	ASN	497	109.829	57.853	60.443	1.00	19.49	B	N
ATOM	9782	C	ASN	497	110.373	58.292	65.193	1.00	17.71	B	C
ATOM	9783	O	ASN	497	109.591	57.420	65.564	1.00	19.20	B	O
ATOM	9784	N	SER	498	111.179	58.924	66.035	1.00	18.90	B	N
ATOM	9785	CA	SER	498	111.147	58.627	67.458	1.00	20.75	B	C
ATOM	9786	CB	SER	498	112.210	59.454	68.191	1.00	20.93	B	C
ATOM	9787	OG	SER	498	113.491	58.878	68.037	1.00	23.33	B	O
ATOM	9788	C	SER	498	109.760	58.956	68.020	1.00	20.54	B	C
ATOM	9789	O	SER	498	109.183	58.184	68.777	1.00	20.68	B	O
ATOM	9790	N	ALA	499	109.238	60.113	67.637	1.00	20.46	B	N
ATOM	9791	CA	ALA	499	107.935	60.564	68.087	1.00	21.87	B	C
ATOM	9792	CB	ALA	499	107.577	61.858	67.391	1.00	21.73	B	C
ATOM	9793	C	ALA	499	106.859	59.520	67.822	1.00	23.85	B	C
ATOM	9794	O	ALA	499	106.279	58.961	68.758	1.00	25.77	B	O
ATOM	9795	N	LEU	500	106.588	59.262	66.546	1.00	23.83	B	N
ATOM	9796	CA	LEU	500	105.568	58.286	66.176	1.00	24.31	B	C
ATOM	9797	CB	LEU	500	105.642	57.958	64.678	1.00	22.08	B	C
ATOM	9798	CG	LEU	500	104.618	56.922	64.201	1.00	20.35	B	C
ATOM	9799	CD1	LEU	500	103.200	57.349	64.570	1.00	19.30	B	C

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## FIG. 4 - 201

(Continued)

ATOM	9800	CD2	LEU	500	104.744	56.763	62.721	1.00	19.60	B	C
ATOM	9801	C	LEU	500	105.745	57.009	66.974	1.00	24.37	B	C
ATOM	9802	O	LEU	500	104.777	56.407	67.437	1.00	24.06	B	O
ATOM	9803	N	ASP	501	106.997	56.601	67.131	1.00	26.06	B	N
ATOM	9804	CA	ASP	501	107.301	55.392	67.868	1.00	26.81	B	C
ATOM	9805	CB	ASP	501	108.793	55.120	67.844	1.00	25.74	B	C
ATOM	9806	CG	ASP	501	109.145	53.848	68.556	1.00	26.66	B	C
ATOM	9807	OD1	ASP	501	108.621	52.789	68.164	1.00	29.87	B	O
ATOM	9808	OD2	ASP	501	109.939	53.901	69.512	1.00	30.35	B	O
ATOM	9809	C	ASP	501	106.827	55.484	69.309	1.00	27.60	B	C
ATOM	9810	O	ASP	501	106.296	54.520	69.855	1.00	27.99	B	O
ATOM	9811	N	LYS	502	107.011	56.645	69.924	1.00	28.69	B	N
ATOM	9812	CA	LYS	502	106.591	56.819	71.301	1.00	31.12	B	C
ATOM	9813	CB	LYS	502	107.034	58.184	71.834	1.00	33.97	B	C
ATOM	9814	CG	LYS	502	106.507	58.484	73.239	1.00	35.56	B	C
ATOM	9815	CD	LYS	502	106.991	59.822	73.766	1.00	36.56	B	C
ATOM	9816	CE	LYS	502	106.308	60.162	75.083	1.00	37.47	B	C
ATOM	9817	NZ	LYS	502	106.514	59.098	76.104	1.00	38.22	B	N
ATOM	9818	C	LYS	502	105.080	56.679	71.426	1.00	31.95	B	C
ATOM	9819	O	LYS	502	104.592	55.937	72.276	1.00	33.49	B	O
ATOM	9820	N	MET	503	104.338	57.380	70.574	1.00	32.49	B	N
ATOM	9821	CA	MET	503	102.881	57.307	70.624	1.00	33.25	B	C
ATOM	9822	CB	MET	503	102.254	58.342	69.690	1.00	35.92	B	C
ATOM	9823	CG	MET	503	102.518	59.768	70.131	1.00	42.44	B	C
ATOM	9824	SD	MET	503	101.702	60.993	69.105	1.00	52.16	B	S
ATOM	9825	CE	MET	503	100.419	61.581	70.243	1.00	50.62	B	C
ATOM	9826	C	MET	503	102.361	55.927	70.279	1.00	31.30	B	C
ATOM	9827	O	MET	503	101.476	55.413	70.954	1.00	31.92	B	O
ATOM	9828	N	LEU	504	102.914	55.318	69.238	1.00	30.00	B	N
ATOM	9829	CA	LEU	504	102.471	53.993	68.836	1.00	29.48	B	C
ATOM	9830	CB	LEU	504	103.276	53.517	67.624	1.00	28.63	B	C
ATOM	9831	CG	LEU	504	102.517	53.477	66.290	1.00	29.55	B	C
ATOM	9832	CD1	LEU	504	101.696	54.750	66.106	1.00	28.10	B	C
ATOM	9833	CD2	LEU	504	103.508	53.300	65.143	1.00	27.73	B	C
ATOM	9834	C	LEU	504	102.581	52.998	69.986	1.00	29.56	B	C
ATOM	9835	O	LEU	504	101.880	51.991	70.016	1.00	27.71	B	O
ATOM	9836	N	GLN	505	103.458	53.291	70.938	1.00	31.52	B	N
ATOM	9837	CA	GLN	505	103.641	52.425	72.096	1.00	33.96	B	C
ATOM	9838	CB	GLN	505	104.829	52.915	72.927	1.00	36.96	B	C
ATOM	9839	CG	GLN	505	106.167	52.836	72.200	1.00	42.44	B	C
ATOM	9840	CD	GLN	505	106.652	51.408	71.996	1.00	43.93	B	C
ATOM	9841	OE1	GLN	505	107.079	50.746	72.943	1.00	45.80	B	O
ATOM	9842	NE2	GLN	505	106.581	50.925	70.758	1.00	45.49	B	N
ATOM	9843	C	GLN	505	102.375	52.393	72.960	1.00	33.38	B	C
ATOM	9844	O	GLN	505	102.104	51.400	73.634	1.00	32.77	B	O
ATOM	9845	N	ASN	506	101.607	53.482	72.928	1.00	32.89	B	N
ATOM	9846	CA	ASN	506	100.362	53.590	73.694	1.00	32.38	B	C
ATOM	9847	CB	ASN	506	99.997	55.062	73.937	1.00	35.05	B	C
ATOM	9848	CG	ASN	506	101.108	55.848	74.629	1.00	39.34	B	C

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(Continued)

## FIG. 4 - 202

ATOM	9849	OD1	ASN	506	101.426	55.608	75.799	1.00	41.09	B	O
ATOM	9850	ND2	ASN	506	101.703	56.796	73.903	1.00	39.00	B	N
ATOM	9851	C	ASN	506	99.208	52.933	72.936	1.00	30.32	B	C
ATOM	9852	O	ASN	506	98.058	52.995	73.377	1.00	30.93	B	O
ATOM	9853	N	VAL	507	99.516	52.305	71.803	1.00	26.94	B	N
ATOM	9854	CA	VAL	507	98.497	51.664	70.974	1.00	25.15	B	C
ATOM	9855	CB	VAL	507	98.456	52.293	69.545	1.00	23.88	B	C
ATOM	9856	CG1	VAL	507	97.287	51.730	68.755	1.00	21.31	B	C
ATOM	9857	CG2	VAL	507	98.344	53.811	69.633	1.00	22.11	B	C
ATOM	9858	C	VAL	507	98.717	50.164	70.825	1.00	25.62	B	C
ATOM	9859	O	VAL	507	99.838	49.676	70.945	1.00	26.78	B	O
ATOM	9860	N	GLN	508	97.639	49.432	70.567	1.00	25.89	B	N
ATOM	9861	CA	GLN	508	97.730	47.992	70.381	1.00	25.14	B	C
ATOM	9862	CB	GLN	508	96.486	47.281	70.917	1.00	27.32	B	C
ATOM	9863	CG	GLN	508	96.322	47.397	72.422	1.00	29.65	B	C
ATOM	9864	CD	GLN	508	95.190	46.543	72.958	1.00	30.81	B	C
ATOM	9865	OE1	GLN	508	95.208	45.312	72.836	1.00	31.32	B	O
ATOM	9866	NE2	GLN	508	94.199	47.190	73.561	1.00	29.92	B	N
ATOM	9867	C	GLN	508	97.869	47.740	68.899	1.00	23.65	B	C
ATOM	9868	O	GLN	508	96.944	47.277	68.241	1.00	22.60	B	O
ATOM	9869	N	MET	509	99.046	48.063	68.385	1.00	23.78	B	N
ATOM	9870	CA	MET	509	99.347	47.895	66.980	1.00	23.48	B	C
ATOM	9871	CB	MET	509	100.667	48.578	66.655	1.00	23.41	B	C
ATOM	9872	CG	MET	509	100.586	50.070	66.782	1.00	26.19	B	C
ATOM	9873	SD	MET	509	99.279	50.681	65.719	1.00	28.03	B	S
ATOM	9874	CE	MET	509	100.207	50.994	64.209	1.00	25.78	B	C
ATOM	9875	C	MET	509	99.425	46.440	66.579	1.00	23.44	B	C
ATOM	9876	O	MET	509	99.902	45.599	67.343	1.00	24.15	B	O
ATOM	9877	N	PRO	510	98.951	46.121	65.365	1.00	22.69	B	N
ATOM	9878	CD	PRO	510	98.308	47.027	64.395	1.00	22.87	B	C
ATOM	9879	CA	PRO	510	98.974	44.751	64.854	1.00	21.97	B	C
ATOM	9880	CB	PRO	510	97.987	44.807	63.701	1.00	22.62	B	C
ATOM	9881	CG	PRO	510	98.248	46.171	63.141	1.00	22.72	B	C
ATOM	9882	C	PRO	510	100.381	44.434	64.379	1.00	21.20	B	C
ATOM	9883	O	PRO	510	101.249	45.301	64.353	1.00	19.97	B	O
ATOM	9884	N	SER	511	100.605	43.188	63.997	1.00	22.07	B	N
ATOM	9885	CA	SER	511	101.916	42.782	63.521	1.00	23.02	B	C
ATOM	9886	CB	SER	511	102.481	41.654	64.392	1.00	23.03	B	C
ATOM	9887	OG	SER	511	101.653	40.500	64.358	1.00	26.12	B	O
ATOM	9888	C	SER	511	101.773	42.299	62.094	1.00	23.35	B	C
ATOM	9889	O	SER	511	100.659	42.168	61.583	1.00	24.92	B	O
ATOM	9890	N	LYS	512	102.906	42.035	61.458	1.00	22.83	B	N
ATOM	9891	CA	LYS	512	102.916	41.556	60.094	1.00	22.46	B	C
ATOM	9892	CB	LYS	512	103.490	42.615	59.168	1.00	21.81	B	C
ATOM	9893	CG	LYS	512	103.494	42.209	57.705	1.00	23.24	B	C
ATOM	9894	CD	LYS	512	103.820	43.411	56.851	1.00	24.28	B	C
ATOM	9895	CE	LYS	512	103.824	43.080	55.393	1.00	23.13	B	C
ATOM	9896	NZ	LYS	512	104.160	44.299	54.622	1.00	24.52	B	N
ATOM	9897	C	LYS	512	103.742	40.289	59.993	1.00	22.87	B	C

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## FIG. 4 - 203

(Continued)

ATOM	9898	O	LYS	512	104.803	40.180	60.585	1.00	23.26	B	O
ATOM	9899	N	LYS	513	103.235	39.331	59.235	1.00	24.10	B	N
ATOM	9900	CA	LYS	513	103.910	38.069	59.039	1.00	24.49	B	C
ATOM	9901	CB	LYS	513	103.046	36.923	59.566	1.00	25.52	B	C
ATOM	9902	CG	LYS	513	103.522	35.537	59.148	1.00	26.69	B	C
ATOM	9903	CD	LYS	513	102.493	34.471	59.522	1.00	30.85	B	C
ATOM	9904	CE	LYS	513	102.805	33.124	58.866	1.00	33.37	B	C
ATOM	9905	NZ	LYS	513	104.131	32.573	59.287	1.00	36.04	B	N
ATOM	9906	C	LYS	513	104.143	37.888	57.552	1.00	25.44	B	C
ATOM	9907	O	LYS	513	103.196	37.871	56.763	1.00	27.00	B	O
ATOM	9908	N	LEU	514	105.409	37.771	57.171	1.00	24.62	B	N
ATOM	9909	CA	LEU	514	105.775	37.561	55.783	1.00	22.99	B	C
ATOM	9910	CB	LEU	514	106.870	38.536	55.380	1.00	22.15	B	C
ATOM	9911	CG	LEU	514	107.307	38.465	53.925	1.00	21.19	B	C
ATOM	9912	CD1	LEU	514	106.125	38.790	53.029	1.00	19.85	B	C
ATOM	9913	CD2	LEU	514	108.438	39.435	53.701	1.00	18.42	B	C
ATOM	9914	C	LEU	514	106.292	36.132	55.708	1.00	24.30	B	C
ATOM	9915	O	LEU	514	107.123	35.725	56.519	1.00	24.87	B	O
ATOM	9916	N	ASP	515	105.804	35.361	54.747	1.00	25.31	B	N
ATOM	9917	CA	ASP	515	106.233	33.975	54.634	1.00	26.30	B	C
ATOM	9918	CB	ASP	515	105.599	33.156	55.757	1.00	28.58	B	C
ATOM	9919	CG	ASP	515	106.403	31.929	56.108	1.00	30.08	B	C
ATOM	9920	OD1	ASP	515	107.209	31.474	55.272	1.00	31.89	B	O
ATOM	9921	OD2	ASP	515	106.216	31.409	57.224	1.00	33.36	B	O
ATOM	9922	C	ASP	515	105.805	33.414	53.282	1.00	26.17	B	C
ATOM	9923	O	ASP	515	105.343	34.157	52.417	1.00	26.57	B	O
ATOM	9924	N	PHE	516	105.940	32.104	53.103	1.00	25.46	B	N
ATOM	9925	CA	PHE	516	105.571	31.496	51.838	1.00	25.82	B	C
ATOM	9926	CB	PHE	516	106.792	31.384	50.930	1.00	23.83	B	C
ATOM	9927	CG	PHE	516	107.811	30.395	51.413	1.00	22.29	B	C
ATOM	9928	CD1	PHE	516	108.896	30.808	52.176	1.00	22.68	B	C
ATOM	9929	CD2	PHE	516	107.678	29.042	51.119	1.00	21.58	B	C
ATOM	9930	CE1	PHE	516	109.836	29.885	52.642	1.00	21.89	B	C
ATOM	9931	CE2	PHE	516	108.609	28.113	51.579	1.00	21.19	B	C
ATOM	9932	CZ	PHE	516	109.689	28.536	52.342	1.00	20.70	B	C
ATOM	9933	C	PHE	516	104.955	30.117	51.954	1.00	26.95	B	C
ATOM	9934	O	PHE	516	105.063	29.452	52.980	1.00	28.94	B	O
ATOM	9935	N	ILE	517	104.307	29.707	50.872	1.00	27.35	B	N
ATOM	9936	CA	ILE	517	103.697	28.398	50.755	1.00	28.12	B	C
ATOM	9937	CB	ILE	517	102.155	28.470	50.729	1.00	26.53	B	C
ATOM	9938	CG2	ILE	517	101.645	29.073	52.016	1.00	27.39	B	C
ATOM	9939	CG1	ILE	517	101.682	29.296	49.537	1.00	27.43	B	C
ATOM	9940	CD1	ILE	517	100.175	29.486	49.486	1.00	26.37	B	C
ATOM	9941	C	ILE	517	104.202	27.896	49.411	1.00	30.13	B	C
ATOM	9942	O	ILE	517	104.575	28.697	48.551	1.00	29.21	B	O
ATOM	9943	N	ILE	518	104.239	26.581	49.228	1.00	33.16	B	N
ATOM	9944	CA	ILE	518	104.709	26.029	47.969	1.00	36.01	B	C
ATOM	9945	CB	ILE	518	105.680	24.867	48.190	1.00	36.84	B	C
ATOM	9946	CG2	ILE	518	106.133	24.311	46.845	1.00	36.94	B	C

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(Continued)

## FIG. 4 - 204

ATOM	9947	CG1	ILE	518	106.884	25.349	49.000	1.00	38.21	B	C
ATOM	9948	CD1	ILE	518	107.976	24.296	49.169	1.00	40.77	B	C
ATOM	9949	C	ILE	518	103.558	25.534	47.114	1.00	37.38	B	C
ATOM	9950	O	ILE	518	102.581	25.000	47.624	1.00	38.97	B	O
ATOM	9951	N	LEU	519	103.679	25.730	45.808	1.00	39.11	B	N
ATOM	9952	CA	LEU	519	102.663	25.294	44.863	1.00	40.68	B	C
ATOM	9953	CB	LEU	519	101.753	26.461	44.474	1.00	39.71	B	C
ATOM	9954	CG	LEU	519	100.989	27.144	45.612	1.00	39.82	B	C
ATOM	9955	CD1	LEU	519	100.051	28.205	45.045	1.00	39.14	B	C
ATOM	9956	CD2	LEU	519	100.194	26.107	46.381	1.00	40.51	B	C
ATOM	9957	C	LEU	519	103.388	24.763	43.637	1.00	42.22	B	C
ATOM	9958	O	LEU	519	104.028	25.524	42.910	1.00	42.60	B	O
ATOM	9959	N	ASN	520	103.299	23.453	43.419	1.00	43.53	B	N
ATOM	9960	CA	ASN	520	103.963	22.824	42.285	1.00	44.57	B	C
ATOM	9961	CB	ASN	520	103.385	23.337	40.964	1.00	46.39	B	C
ATOM	9962	CG	ASN	520	102.045	22.726	40.639	1.00	48.97	B	C
ATOM	9963	OD1	ASN	520	101.168	22.634	41.498	1.00	50.54	B	O
ATOM	9964	ND2	ASN	520	101.871	22.312	39.386	1.00	50.46	B	N
ATOM	9965	C	ASN	520	105.452	23.114	42.316	1.00	44.13	B	C
ATOM	9966	O	ASN	520	106.004	23.637	41.348	1.00	44.64	B	O
ATOM	9967	N	GLU	521	106.097	22.791	43.431	1.00	44.10	B	N
ATOM	9968	CA	GLU	521	107.536	23.012	43.562	1.00	45.15	B	C
ATOM	9969	CB	GLU	521	108.272	22.387	42.368	1.00	49.07	B	C
ATOM	9970	CG	GLU	521	109.775	22.642	42.339	1.00	54.49	B	C
ATOM	9971	CD	GLU	521	110.401	22.274	41.004	1.00	58.04	B	C
ATOM	9972	OE1	GLU	521	110.307	21.091	40.597	1.00	59.07	B	O
ATOM	9973	OE2	GLU	521	110.986	23.176	40.361	1.00	59.78	B	O
ATOM	9974	C	GLU	521	107.922	24.486	43.661	1.00	42.18	B	C
ATOM	9975	O	GLU	521	109.034	24.810	44.072	1.00	42.85	B	O
ATOM	9976	N	THR	522	107.014	25.378	43.283	1.00	38.59	B	N
ATOM	9977	CA	THR	522	107.314	26.800	43.333	1.00	34.63	B	C
ATOM	9978	CB	THR	522	106.605	27.566	42.198	1.00	34.21	B	C
ATOM	9979	OG1	THR	522	107.109	27.115	40.936	1.00	34.20	B	O
ATOM	9980	CG2	THR	522	106.866	29.057	42.318	1.00	33.69	B	C
ATOM	9981	C	THR	522	106.959	27.441	44.664	1.00	32.83	B	C
ATOM	9982	O	THR	522	106.028	27.027	45.350	1.00	32.75	B	O
ATOM	9983	N	LYS	523	107.727	28.464	45.011	1.00	31.06	B	N
ATOM	9984	CA	LYS	523	107.559	29.206	46.245	1.00	29.30	B	C
ATOM	9985	CB	LYS	523	108.940	29.490	46.838	1.00	29.00	B	C
ATOM	9986	CG	LYS	523	108.934	30.329	48.089	1.00	31.42	B	C
ATOM	9987	CD	LYS	523	110.344	30.567	48.607	1.00	32.07	B	C
ATOM	9988	CE	LYS	523	111.045	29.265	48.943	1.00	33.13	B	C
ATOM	9989	NZ	LYS	523	112.388	29.512	49.545	1.00	35.72	B	N
ATOM	9990	C	LYS	523	106.819	30.519	45.984	1.00	28.56	B	C
ATOM	9991	O	LYS	523	107.256	31.335	45.173	1.00	29.36	B	O
ATOM	9992	N	PHE	524	105.692	30.711	46.661	1.00	25.40	B	N
ATOM	9993	CA	PHE	524	104.912	31.934	46.517	1.00	22.61	B	C
ATOM	9994	CB	PHE	524	103.529	31.637	45.929	1.00	22.69	B	C
ATOM	9995	CG	PHE	524	103.565	31.136	44.516	1.00	21.75	B	C

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## FIG. 4 - 205

(Continued)

ATOM	9996	CD1	PHE	524	103.626	29.773	44.247	1.00	22.19	B	C
ATOM	9997	CD2	PHE	524	103.541	32.031	43.448	1.00	22.40	B	C
ATOM	9998	CE1	PHE	524	103.662	29.306	42.935	1.00	22.45	B	C
ATOM	9999	CE2	PHE	524	103.576	31.579	42.131	1.00	22.01	B	C
ATOM	10000	CZ	PHE	524	103.637	30.213	41.871	1.00	22.70	B	C
ATOM	10001	C	PHE	524	104.765	32.593	47.890	1.00	20.73	B	C
ATOM	10002	O	PHE	524	104.416	31.941	48.875	1.00	19.19	B	O
ATOM	10003	N	TRP	525	105.016	33.892	47.950	1.00	18.35	B	N
ATOM	10004	CA	TRP	525	104.950	34.600	49.216	1.00	17.31	B	C
ATOM	10005	CB	TRP	525	106.059	35.646	49.274	1.00	16.81	B	C
ATOM	10006	CG	TRP	525	107.442	35.092	49.191	1.00	16.14	B	C
ATOM	10007	CD2	TRP	525	108.393	35.031	50.253	1.00	14.70	B	C
ATOM	10008	CE2	TRP	525	109.574	34.454	49.726	1.00	16.70	B	C
ATOM	10009	CE3	TRP	525	108.366	35.411	51.602	1.00	14.22	B	C
ATOM	10010	CD1	TRP	525	108.062	34.560	48.086	1.00	15.59	B	C
ATOM	10011	NE1	TRP	525	109.344	34.176	48.403	1.00	14.99	B	N
ATOM	10012	CZ2	TRP	525	110.722	34.247	50.508	1.00	17.11	B	C
ATOM	10013	CZ3	TRP	525	109.506	35.204	52.381	1.00	14.40	B	C
ATOM	10014	CH2	TRP	525	110.668	34.627	51.829	1.00	15.16	B	C
ATOM	10015	C	TRP	525	103.630	35.280	49.554	1.00	17.78	B	C
ATOM	10016	O	TRP	525	102.880	35.719	48.675	1.00	17.96	B	O
ATOM	10017	N	TYR	526	103.361	35.368	50.849	1.00	16.97	B	N
ATOM	10018	CA	TYR	526	102.165	36.034	51.341	1.00	18.30	B	C
ATOM	10019	CB	TYR	526	101.053	35.030	51.652	1.00	19.10	B	C
ATOM	10020	CG	TYR	526	101.369	34.076	52.778	1.00	21.69	B	C
ATOM	10021	CD1	TYR	526	101.132	34.422	54.110	1.00	23.52	B	C
ATOM	10022	CE1	TYR	526	101.416	33.531	55.146	1.00	25.02	B	C
ATOM	10023	CD2	TYR	526	101.902	32.817	52.509	1.00	24.93	B	C
ATOM	10024	CE2	TYR	526	102.189	31.922	53.527	1.00	26.65	B	C
ATOM	10025	CZ	TYR	526	101.945	32.280	54.840	1.00	28.49	B	C
ATOM	10026	OH	TYR	526	102.235	31.370	55.830	1.00	31.26	B	O
ATOM	10027	C	TYR	526	102.540	36.770	52.609	1.00	16.76	B	C
ATOM	10028	O	TYR	526	103.600	36.536	53.187	1.00	15.11	B	O
ATOM	10029	N	GLN	527	101.676	37.680	53.024	1.00	17.09	B	N
ATOM	10030	CA	GLN	527	101.901	38.417	54.250	1.00	17.75	B	C
ATOM	10031	CB	GLN	527	102.417	39.833	53.978	1.00	16.32	B	C
ATOM	10032	CG	GLN	527	101.462	40.740	53.234	1.00	15.60	B	C
ATOM	10033	CD	GLN	527	101.935	42.188	53.213	1.00	16.43	B	C
ATOM	10034	OE1	GLN	527	103.016	42.502	52.707	1.00	13.50	B	O
ATOM	10035	NE2	GLN	527	101.121	43.079	53.771	1.00	15.38	B	N
ATOM	10036	C	GLN	527	100.556	38.477	54.930	1.00	19.32	B	C
ATOM	10037	O	GLN	527	99.519	38.439	54.269	1.00	19.02	B	O
ATOM	10038	N	MET	528	100.575	38.532	56.253	1.00	20.93	B	N
ATOM	10039	CA	MET	528	99.346	38.608	57.018	1.00	21.02	B	C
ATOM	10040	CB	MET	528	99.076	37.295	57.748	1.00	21.14	B	C
ATOM	10041	CG	MET	528	98.575	36.178	56.859	1.00	23.54	B	C
ATOM	10042	SD	MET	528	98.325	34.650	57.776	1.00	23.43	B	S
ATOM	10043	CE	MET	528	96.628	34.772	58.155	1.00	26.01	B	C
ATOM	10044	C	MET	528	99.458	39.720	58.033	1.00	20.94	B	C

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## FIG. 4 - 206

(Continued)

ATOM	10045	O	MET	528	100.471	39.845	58.720	1.00	21.07	B	O
ATOM	10046	N	ILE	529	98.432	40.554	58.100	1.00	19.01	B	N
ATOM	10047	CA	ILE	529	98.428	41.614	59.082	1.00	18.89	B	C
ATOM	10048	CB	ILE	529	97.718	42.860	58.540	1.00	16.80	B	C
ATOM	10049	CG2	ILE	529	97.656	43.937	59.615	1.00	13.98	B	C
ATOM	10050	CG1	ILE	529	98.469	43.368	57.296	1.00	15.06	B	C
ATOM	10051	CD1	ILE	529	99.934	43.701	57.537	1.00	11.03	B	C
ATOM	10052	C	ILE	529	97.656	40.969	60.225	1.00	20.15	B	C
ATOM	10053	O	ILE	529	96.457	40.720	60.124	1.00	20.94	B	O
ATOM	10054	N	LEU	530	98.359	40.653	61.302	1.00	21.19	B	N
ATOM	10055	CA	LEU	530	97.717	39.985	62.420	1.00	21.61	B	C
ATOM	10056	CB	LEU	530	98.649	38.907	62.976	1.00	19.85	B	C
ATOM	10057	CG	LEU	530	99.086	37.875	61.931	1.00	19.34	B	C
ATOM	10058	CD1	LEU	530	100.238	37.027	62.461	1.00	20.33	B	C
ATOM	10059	CD2	LEU	530	97.897	37.010	61.562	1.00	19.04	B	C
ATOM	10060	C	LEU	530	97.294	40.930	63.521	1.00	22.34	B	C
ATOM	10061	O	LEU	530	98.006	41.878	63.854	1.00	23.45	B	O
ATOM	10062	N	PRO	531	96.104	40.697	64.088	1.00	23.19	B	N
ATOM	10063	CD	PRO	531	95.105	39.684	63.711	1.00	22.71	B	C
ATOM	10064	CA	PRO	531	95.600	41.545	65.169	1.00	24.33	B	C
ATOM	10065	CB	PRO	531	94.188	41.002	65.404	1.00	22.74	B	C
ATOM	10066	CG	PRO	531	94.276	39.588	64.967	1.00	23.03	B	C
ATOM	10067	C	PRO	531	96.490	41.438	66.407	1.00	25.18	B	C
ATOM	10068	O	PRO	531	97.244	40.478	66.562	1.00	24.64	B	O
ATOM	10069	N	PRO	532	96.424	42.433	67.300	1.00	26.64	B	N
ATOM	10070	CD	PRO	532	95.502	43.581	67.326	1.00	25.36	B	C
ATOM	10071	CA	PRO	532	97.246	42.397	68.513	1.00	27.91	B	C
ATOM	10072	CB	PRO	532	96.868	43.698	69.216	1.00	27.08	B	C
ATOM	10073	CG	PRO	532	95.443	43.897	68.793	1.00	26.25	B	C
ATOM	10074	C	PRO	532	96.945	41.160	69.369	1.00	29.25	B	C
ATOM	10075	O	PRO	532	95.865	40.579	69.279	1.00	29.62	B	O
ATOM	10076	N	HIS	533	97.909	40.756	70.187	1.00	30.65	B	N
ATOM	10077	CA	HIS	533	97.738	39.602	71.061	1.00	31.99	B	C
ATOM	10078	CB	HIS	533	96.749	39.945	72.172	1.00	32.50	B	C
ATOM	10079	CG	HIS	533	96.981	41.293	72.783	1.00	35.12	B	C
ATOM	10080	CD2	HIS	533	96.168	42.370	72.903	1.00	36.18	B	C
ATOM	10081	ND1	HIS	533	98.181	41.653	73.358	1.00	35.49	B	N
ATOM	10082	CE1	HIS	533	98.096	42.892	73.807	1.00	36.37	B	C
ATOM	10083	NE2	HIS	533	96.885	43.350	73.544	1.00	37.01	B	N
ATOM	10084	C	HIS	533	97.249	38.382	70.286	1.00	33.21	B	C
ATOM	10085	O	HIS	533	96.447	37.590	70.791	1.00	32.78	B	O
ATOM	10086	N	PHE	534	97.739	38.243	69.058	1.00	33.50	B	N
ATOM	10087	CA	PHE	534	97.374	37.125	68.200	1.00	34.63	B	C
ATOM	10088	CB	PHE	534	98.283	37.085	66.970	1.00	32.35	B	C
ATOM	10089	CG	PHE	534	97.997	35.942	66.041	1.00	32.06	B	C
ATOM	10090	CD1	PHE	534	96.790	35.871	65.354	1.00	32.10	B	C
ATOM	10091	CD2	PHE	534	98.936	34.938	65.848	1.00	32.66	B	C
ATOM	10092	CE1	PHE	534	96.522	34.819	64.486	1.00	31.59	B	C
ATOM	10093	CE2	PHE	534	98.679	33.879	64.982	1.00	32.91	B	C

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## FIG. 4 - 207

(Continued)

ATOM	10094	CZ	PHE	534	97.469	33.820	64.298	1.00	32.93	B	C
ATOM	10095	C	PHE	534	97.503	35.806	68.941	1.00	36.77	B	C
ATOM	10096	O	PHE	534	98.532	35.534	69.565	1.00	37.84	B	O
ATOM	10097	N	ASP	535	96.463	34.982	68.868	1.00	39.07	B	N
ATOM	10098	CA	ASP	535	96.480	33.680	69.523	1.00	40.37	B	C
ATOM	10099	CB	ASP	535	95.458	33.639	70.655	1.00	42.55	B	C
ATOM	10100	CG	ASP	535	95.544	32.363	71.465	1.00	45.66	B	C
ATOM	10101	OD1	ASP	535	94.783	32.227	72.445	1.00	49.45	B	O
ATOM	10102	OD2	ASP	535	96.372	31.494	71.125	1.00	46.59	B	O
ATOM	10103	C	ASP	535	96.159	32.601	68.503	1.00	39.36	B	C
ATOM	10104	O	ASP	535	95.047	32.540	67.996	1.00	39.17	B	O
ATOM	10105	N	LYS	536	97.135	31.746	68.216	1.00	40.23	B	N
ATOM	10106	CA	LYS	536	96.964	30.680	67.233	1.00	41.20	B	C
ATOM	10107	CB	LYS	536	98.302	30.001	66.947	1.00	42.62	B	C
ATOM	10108	CG	LYS	536	98.266	29.089	65.731	1.00	46.75	B	C
ATOM	10109	CD	LYS	536	99.657	28.577	65.355	1.00	49.06	B	C
ATOM	10110	CE	LYS	536	99.624	27.800	64.040	1.00	48.68	B	C
ATOM	10111	NZ	LYS	536	98.648	26.676	64.079	1.00	48.77	B	N
ATOM	10112	C	LYS	536	95.937	29.620	67.607	1.00	40.95	B	C
ATOM	10113	O	LYS	536	95.577	28.785	66.778	1.00	41.99	B	O
ATOM	10114	N	SER	537	95.464	29.649	68.848	1.00	40.73	B	N
ATOM	10115	CA	SER	537	94.469	28.681	69.296	1.00	40.33	B	C
ATOM	10116	CB	SER	537	94.598	28.438	70.805	1.00	40.23	B	C
ATOM	10117	OG	SER	537	94.434	29.636	71.541	1.00	40.12	B	O
ATOM	10118	C	SER	537	93.064	29.179	68.968	1.00	40.20	B	C
ATOM	10119	O	SER	537	92.103	28.412	68.977	1.00	40.87	B	O
ATOM	10120	N	LYS	538	92.951	30.469	68.674	1.00	39.23	B	N
ATOM	10121	CA	LYS	538	91.666	31.067	68.337	1.00	37.32	B	C
ATOM	10122	CB	LYS	538	91.629	32.517	68.817	1.00	39.07	B	C
ATOM	10123	CG	LYS	538	92.298	32.747	70.170	1.00	41.74	B	C
ATOM	10124	CD	LYS	538	91.534	32.100	71.316	1.00	44.86	B	C
ATOM	10125	CE	LYS	538	90.186	32.773	71.540	1.00	46.82	B	C
ATOM	10126	NZ	LYS	538	89.417	32.121	72.636	1.00	47.36	B	N
ATOM	10127	C	LYS	538	91.507	31.028	66.819	1.00	35.00	B	C
ATOM	10128	O	LYS	538	92.464	30.754	66.101	1.00	34.33	B	O
ATOM	10129	N	LYS	539	90.299	31.288	66.335	1.00	33.57	B	N
ATOM	10130	CA	LYS	539	90.038	31.302	64.895	1.00	32.92	B	C
ATOM	10131	CB	LYS	539	89.049	30.197	64.510	1.00	32.99	B	C
ATOM	10132	CG	LYS	539	89.736	28.887	64.143	1.00	36.07	B	C
ATOM	10133	CD	LYS	539	88.757	27.739	63.893	1.00	39.32	B	C
ATOM	10134	CE	LYS	539	87.720	28.059	62.816	1.00	39.62	B	C
ATOM	10135	NZ	LYS	539	86.644	28.969	63.310	1.00	39.49	B	N
ATOM	10136	C	LYS	539	89.504	32.666	64.471	1.00	31.07	B	C
ATOM	10137	O	LYS	539	88.424	33.087	64.902	1.00	30.44	B	O
ATOM	10138	N	TYR	540	90.274	33.356	63.633	1.00	27.48	B	N
ATOM	10139	CA	TYR	540	89.893	34.682	63.165	1.00	24.82	B	C
ATOM	10140	CB	TYR	540	91.096	35.624	63.178	1.00	23.82	B	C
ATOM	10141	CG	TYR	540	91.849	35.702	64.482	1.00	23.61	B	C
ATOM	10142	CD1	TYR	540	92.614	34.627	64.936	1.00	21.98	B	C

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(Continued)

## FIG. 4 - 208

ATOM	10143	CE1	TYR	540	93.321	34.708	66.130	1.00	21.65	B	C
ATOM	10144	CD2	TYR	540	91.810	36.863	65.257	1.00	22.89	B	C
ATOM	10145	CE2	TYR	540	92.507	36.955	66.449	1.00	22.77	B	C
ATOM	10146	CZ	TYR	540	93.261	35.875	66.881	1.00	22.87	B	C
ATOM	10147	OH	TYR	540	93.950	35.965	68.062	1.00	23.97	B	O
ATOM	10148	C	TYR	540	89.335	34.694	61.749	1.00	23.62	B	C
ATOM	10149	O	TYR	540	89.670	33.842	60.925	1.00	23.93	B	O
ATOM	10150	N	PRO	541	88.457	35.660	61.452	1.00	21.89	B	N
ATOM	10151	CD	PRO	541	87.820	36.667	62.320	1.00	21.22	B	C
ATOM	10152	CA	PRO	541	87.917	35.719	60.095	1.00	20.52	B	C
ATOM	10153	CB	PRO	541	86.770	36.717	60.228	1.00	20.30	B	C
ATOM	10154	CG	PRO	541	87.243	37.629	61.317	1.00	20.36	B	C
ATOM	10155	C	PRO	541	89.077	36.266	59.276	1.00	19.86	B	C
ATOM	10156	O	PRO	541	90.026	36.799	59.841	1.00	19.90	B	O
ATOM	10157	N	LEU	542	89.028	36.147	57.961	1.00	19.38	B	N
ATOM	10158	CA	LEU	542	90.133	36.655	57.169	1.00	18.21	B	C
ATOM	10159	CB	LEU	542	91.027	35.483	56.741	1.00	18.98	B	C
ATOM	10160	CG	LEU	542	92.215	35.768	55.816	1.00	19.24	B	C
ATOM	10161	CD1	LEU	542	93.296	34.721	56.025	1.00	17.89	B	C
ATOM	10162	CD2	LEU	542	91.741	35.775	54.374	1.00	19.31	B	C
ATOM	10163	C	LEU	542	89.677	37.458	55.954	1.00	17.31	B	C
ATOM	10164	O	LEU	542	88.720	37.087	55.282	1.00	18.08	B	O
ATOM	10165	N	LEU	543	90.368	38.564	55.694	1.00	14.81	B	N
ATOM	10166	CA	LEU	543	90.075	39.430	54.559	1.00	13.79	B	C
ATOM	10167	CB	LEU	543	89.816	40.872	55.015	1.00	12.33	B	C
ATOM	10168	CG	LEU	543	89.568	41.892	53.886	1.00	13.71	B	C
ATOM	10169	CD1	LEU	543	88.317	41.497	53.113	1.00	9.91	B	C
ATOM	10170	CD2	LEU	543	89.409	43.294	54.454	1.00	11.87	B	C
ATOM	10171	C	LEU	543	91.273	39.415	53.620	1.00	14.35	B	C
ATOM	10172	O	LEU	543	92.349	39.893	53.966	1.00	14.04	B	O
ATOM	10173	N	LEU	544	91.091	38.866	52.428	1.00	15.02	B	N
ATOM	10174	CA	LEU	544	92.191	38.807	51.480	1.00	16.19	B	C
ATOM	10175	CB	LEU	544	92.006	37.609	50.539	1.00	16.34	B	C
ATOM	10176	CG	LEU	544	93.163	37.231	49.608	1.00	14.93	B	C
ATOM	10177	CD1	LEU	544	94.345	36.752	50.429	1.00	15.36	B	C
ATOM	10178	CD2	LEU	544	92.713	36.128	48.654	1.00	15.79	B	C
ATOM	10179	C	LEU	544	92.276	40.109	50.679	1.00	16.49	B	C
ATOM	10180	O	LEU	544	91.437	40.374	49.819	1.00	17.02	B	O
ATOM	10181	N	ASP	545	93.280	40.925	50.997	1.00	15.13	B	N
ATOM	10182	CA	ASP	545	93.515	42.186	50.306	1.00	14.91	B	C
ATOM	10183	CB	ASP	545	94.479	43.069	51.117	1.00	15.71	B	C
ATOM	10184	CG	ASP	545	94.703	44.434	50.483	1.00	15.88	B	C
ATOM	10185	OD1	ASP	545	94.285	44.641	49.324	1.00	14.36	B	O
ATOM	10186	OD2	ASP	545	95.304	45.304	51.144	1.00	15.41	B	O
ATOM	10187	C	ASP	545	94.175	41.757	49.004	1.00	14.61	B	C
ATOM	10188	O	ASP	545	95.235	41.135	49.014	1.00	13.17	B	O
ATOM	10189	N	VAL	546	93.567	42.098	47.881	1.00	15.03	B	N
ATOM	10190	CA	VAL	546	94.116	41.667	46.614	1.00	17.39	B	C
ATOM	10191	CB	VAL	546	93.199	40.579	46.014	1.00	19.44	B	C

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(Continued)

## FIG. 4 - 209

ATOM	10192	CG1	VAL	546	93.717	40.124	44.647	1.00	17.87	B	C
ATOM	10193	CG2	VAL	546	93.109	39.410	46.983	1.00	20.93	B	C
ATOM	10194	C	VAL	546	94.343	42.722	45.542	1.00	17.09	B	C
ATOM	10195	O	VAL	546	93.601	43.694	45.447	1.00	18.12	B	O
ATOM	10196	N	TYR	547	95.391	42.519	44.745	1.00	15.70	B	N
ATOM	10197	CA	TYR	547	95.670	43.378	43.595	1.00	14.90	B	C
ATOM	10198	CB	TYR	547	96.838	44.335	43.821	1.00	12.56	B	C
ATOM	10199	CG	TYR	547	97.008	45.241	42.622	1.00	12.84	B	C
ATOM	10200	CD1	TYR	547	98.064	45.063	41.727	1.00	12.01	B	C
ATOM	10201	CE1	TYR	547	98.165	45.839	40.578	1.00	9.97	B	C
ATOM	10202	CD2	TYR	547	96.057	46.226	42.331	1.00	11.82	B	C
ATOM	10203	CE2	TYR	547	96.149	47.002	41.183	1.00	8.62	B	C
ATOM	10204	CZ	TYR	547	97.204	46.804	40.314	1.00	10.60	B	C
ATOM	10205	OH	TYR	547	97.304	47.573	39.179	1.00	12.10	B	O
ATOM	10206	C	TYR	547	96.011	42.392	42.485	1.00	13.60	B	C
ATOM	10207	O	TYR	547	95.244	42.205	41.548	1.00	13.39	B	O
ATOM	10208	N	ALA	548	97.170	41.763	42.608	1.00	13.66	B	N
ATOM	10209	CA	ALA	548	97.594	40.730	41.672	1.00	14.14	B	C
ATOM	10210	CB	ALA	548	96.658	39.518	41.807	1.00	11.57	B	C
ATOM	10211	C	ALA	548	97.732	41.105	40.207	1.00	13.67	B	C
ATOM	10212	O	ALA	548	97.681	40.234	39.340	1.00	14.21	B	O
ATOM	10213	N	GLY	549	97.905	42.386	39.913	1.00	13.87	B	N
ATOM	10214	CA	GLY	549	98.078	42.765	38.524	1.00	12.26	B	C
ATOM	10215	C	GLY	549	99.405	42.209	38.046	1.00	12.16	B	C
ATOM	10216	O	GLY	549	100.179	41.717	38.855	1.00	12.33	B	O
ATOM	10217	N	PRO	550	99.700	42.256	36.739	1.00	13.98	B	N
ATOM	10218	CD	PRO	550	98.853	42.760	35.644	1.00	12.99	B	C
ATOM	10219	CA	PRO	550	100.969	41.736	36.217	1.00	13.32	B	C
ATOM	10220	CB	PRO	550	100.863	42.007	34.721	1.00	14.56	B	C
ATOM	10221	CG	PRO	550	99.391	42.015	34.473	1.00	14.10	B	C
ATOM	10222	C	PRO	550	102.166	42.459	36.832	1.00	13.86	B	C
ATOM	10223	O	PRO	550	102.248	43.683	36.785	1.00	13.45	B	O
ATOM	10224	N	CYS	551	103.088	41.694	37.405	1.00	14.79	B	N
ATOM	10225	CA	CYS	551	104.283	42.244	38.027	1.00	15.51	B	C
ATOM	10226	CB	CYS	551	105.035	43.139	37.036	1.00	17.05	B	C
ATOM	10227	SG	CYS	551	106.732	43.567	37.543	1.00	17.09	B	S
ATOM	10228	C	CYS	551	103.967	43.018	39.312	1.00	16.05	B	C
ATOM	10229	O	CYS	551	104.693	43.938	39.702	1.00	15.36	B	O
ATOM	10230	N	SER	552	102.883	42.631	39.976	1.00	15.15	B	N
ATOM	10231	CA	SER	552	102.494	43.268	41.229	1.00	14.65	B	C
ATOM	10232	CB	SER	552	100.990	43.149	41.425	1.00	14.47	B	C
ATOM	10233	OG	SER	552	100.604	41.789	41.427	1.00	14.39	B	O
ATOM	10234	C	SER	552	103.201	42.608	42.418	1.00	15.21	B	C
ATOM	10235	O	SER	552	103.882	41.585	42.273	1.00	15.34	B	O
ATOM	10236	N	GLN	553	103.048	43.201	43.594	1.00	14.73	B	N
ATOM	10237	CA	GLN	553	103.654	42.647	44.794	1.00	14.31	B	C
ATOM	10238	CB	GLN	553	105.138	43.017	44.892	1.00	13.21	B	C
ATOM	10239	CG	GLN	553	105.852	42.332	46.056	1.00	15.05	B	C
ATOM	10240	CD	GLN	553	107.359	42.585	46.090	1.00	15.66	B	C

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(Continued)

## FIG. 4 - 210

ATOM	10241	OE1	GLN	553	107.812	43.686	46.400	1.00	16.56	B	O
ATOM	10242	NE2	GLN	553	108.138	41.556	45.773	1.00	15.50	B	N
ATOM	10243	C	GLN	553	102.921	43.166	46.012	1.00	14.58	B	C
ATOM	10244	O	GLN	553	103.148	44.295	46.434	1.00	14.77	B	O
ATOM	10245	N	LYS	554	102.031	42.344	46.568	1.00	14.78	B	N
ATOM	10246	CA	LYS	554	101.284	42.734	47.754	1.00	16.57	B	C
ATOM	10247	CB	LYS	554	99.817	42.318	47.633	1.00	17.81	B	C
ATOM	10248	CG	LYS	554	99.031	43.142	46.630	1.00	18.63	B	C
ATOM	10249	CD	LYS	554	99.047	44.612	47.000	1.00	18.55	B	C
ATOM	10250	CE	LYS	554	98.228	44.902	48.261	1.00	18.33	B	C
ATOM	10251	NZ	LYS	554	96.769	44.771	48.035	1.00	13.33	B	N
ATOM	10252	C	LYS	554	101.890	42.148	49.024	1.00	16.05	B	C
ATOM	10253	O	LYS	554	101.424	42.429	50.124	1.00	17.37	B	O
ATOM	10254	N	ALA	555	102.939	41.350	48.866	1.00	15.91	B	N
ATOM	10255	CA	ALA	555	103.622	40.730	50.004	1.00	15.84	B	C
ATOM	10256	CB	ALA	555	103.656	39.210	49.833	1.00	15.51	B	C
ATOM	10257	C	ALA	555	105.041	41.246	50.142	1.00	14.91	B	C
ATOM	10258	O	ALA	555	105.954	40.691	49.539	1.00	15.57	B	O
ATOM	10259	N	ASP	556	105.233	42.304	50.924	1.00	16.20	B	N
ATOM	10260	CA	ASP	556	106.571	42.854	51.134	1.00	16.65	B	C
ATOM	10261	CB	ASP	556	106.801	44.085	50.243	1.00	17.94	B	C
ATOM	10262	CG	ASP	556	105.750	45.159	50.430	1.00	19.95	B	C
ATOM	10263	OD1	ASP	556	105.355	45.429	51.583	1.00	22.16	B	O
ATOM	10264	OD2	ASP	556	105.327	45.751	49.415	1.00	21.01	B	O
ATOM	10265	C	ASP	556	106.862	43.202	52.597	1.00	16.87	B	C
ATOM	10266	O	ASP	556	106.046	42.962	53.480	1.00	15.15	B	O
ATOM	10267	N	THR	557	108.039	43.762	52.847	1.00	17.93	B	N
ATOM	10268	CA	THR	557	108.443	44.132	54.200	1.00	18.07	B	C
ATOM	10269	CB	THR	557	109.923	43.826	54.396	1.00	18.59	B	C
ATOM	10270	OG1	THR	557	110.687	44.589	53.454	1.00	20.98	B	O
ATOM	10271	CG2	THR	557	110.188	42.358	54.157	1.00	19.55	B	C
ATOM	10272	C	THR	557	108.203	45.616	54.531	1.00	17.89	B	C
ATOM	10273	O	THR	557	108.776	46.151	55.479	1.00	16.94	B	O
ATOM	10274	N	VAL	558	107.348	46.272	53.754	1.00	16.56	B	N
ATOM	10275	CA	VAL	558	107.049	47.682	53.964	1.00	14.93	B	C
ATOM	10276	CB	VAL	558	106.483	48.302	52.676	1.00	14.99	B	C
ATOM	10277	CG1	VAL	558	106.033	49.733	52.940	1.00	13.18	B	C
ATOM	10278	CG2	VAL	558	107.544	48.247	51.568	1.00	13.02	B	C
ATOM	10279	C	VAL	558	106.058	47.921	55.109	1.00	15.99	B	C
ATOM	10280	O	VAL	558	105.060	47.211	55.238	1.00	13.36	B	O
ATOM	10281	N	PHE	559	106.348	48.923	55.941	1.00	15.43	B	N
ATOM	10282	CA	PHE	559	105.484	49.269	57.069	1.00	14.56	B	C
ATOM	10283	CB	PHE	559	106.303	49.933	58.173	1.00	12.72	B	C
ATOM	10284	CG	PHE	559	105.469	50.504	59.282	1.00	11.04	B	C
ATOM	10285	CD1	PHE	559	105.064	49.712	60.347	1.00	10.65	B	C
ATOM	10286	CD2	PHE	559	105.056	51.833	59.244	1.00	12.10	B	C
ATOM	10287	CE1	PHE	559	104.260	50.232	61.356	1.00	8.83	B	C
ATOM	10288	CE2	PHE	559	104.251	52.360	60.252	1.00	10.43	B	C
ATOM	10289	CZ	PHE	559	103.855	51.554	61.307	1.00	8.93	B	C

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## FIG. 4 - 211

(Continued)

ATOM	10290	C	PHE	559	104.395	50.230	56.592	1.00	14.21	B	C
ATOM	10291	O	PHE	559	104.696	51.255	56.000	1.00	14.64	B	O
ATOM	10292	N	ARG	560	103.137	49.907	56.865	1.00	13.77	B	N
ATOM	10293	CA	ARG	560	102.029	50.744	56.421	1.00	14.06	B	C
ATOM	10294	CB	ARG	560	101.354	50.117	55.185	1.00	12.20	B	C
ATOM	10295	CG	ARG	560	102.248	49.988	53.954	1.00	11.36	B	C
ATOM	10296	CD	ARG	560	101.491	49.421	52.755	1.00	10.73	B	C
ATOM	10297	NE	ARG	560	102.322	48.486	51.999	1.00	13.38	B	N
ATOM	10298	CZ	ARG	560	103.126	48.828	51.002	1.00	14.76	B	C
ATOM	10299	NH1	ARG	560	103.203	50.090	50.614	1.00	19.68	B	N
ATOM	10300	NH2	ARG	560	103.887	47.915	50.421	1.00	16.46	B	N
ATOM	10301	C	ARG	560	100.962	50.980	57.486	1.00	14.74	B	C
ATOM	10302	O	ARG	560	100.661	50.100	58.291	1.00	16.54	B	O
ATOM	10303	N	LEU	561	100.403	52.183	57.483	1.00	13.62	B	N
ATOM	10304	CA	LEU	561	99.325	52.551	58.392	1.00	13.55	B	C
ATOM	10305	CB	LEU	561	99.626	53.875	59.100	1.00	11.68	B	C
ATOM	10306	CG	LEU	561	100.694	53.872	60.189	1.00	12.53	B	C
ATOM	10307	CD1	LEU	561	100.901	55.299	60.698	1.00	8.41	B	C
ATOM	10308	CD2	LEU	561	100.275	52.934	61.319	1.00	10.22	B	C
ATOM	10309	C	LEU	561	98.114	52.725	57.475	1.00	12.59	B	C
ATOM	10310	O	LEU	561	97.987	53.734	56.785	1.00	10.30	B	O
ATOM	10311	N	ASN	562	97.222	51.748	57.465	1.00	12.69	B	N
ATOM	10312	CA	ASN	562	96.071	51.841	56.577	1.00	15.06	B	C
ATOM	10313	CB	ASN	562	96.462	51.267	55.220	1.00	14.07	B	C
ATOM	10314	CG	ASN	562	96.924	49.823	55.318	1.00	14.26	B	C
ATOM	10315	OD1	ASN	562	97.566	49.309	54.407	1.00	15.38	B	O
ATOM	10316	ND2	ASN	562	96.582	49.157	56.423	1.00	11.43	B	N
ATOM	10317	C	ASN	562	94.818	51.139	57.086	1.00	14.89	B	C
ATOM	10318	O	ASN	562	94.712	50.793	58.260	1.00	16.50	B	O
ATOM	10319	N	TRP	563	93.872	50.936	56.178	1.00	15.26	B	N
ATOM	10320	CA	TRP	563	92.616	50.281	56.502	1.00	15.35	B	C
ATOM	10321	CB	TRP	563	91.770	50.132	55.244	1.00	13.87	B	C
ATOM	10322	CG	TRP	563	90.365	49.719	55.511	1.00	15.58	B	C
ATOM	10323	CD2	TRP	563	89.623	48.721	54.804	1.00	12.95	B	C
ATOM	10324	CE2	TRP	563	88.330	48.684	55.369	1.00	13.17	B	C
ATOM	10325	CE3	TRP	563	89.927	47.856	53.745	1.00	10.64	B	C
ATOM	10326	CD1	TRP	563	89.512	50.237	56.456	1.00	13.99	B	C
ATOM	10327	NE1	TRP	563	88.289	49.617	56.373	1.00	14.03	B	N
ATOM	10328	CZ2	TRP	563	87.346	47.816	54.911	1.00	13.35	B	C
ATOM	10329	CZ3	TRP	563	88.951	46.995	53.290	1.00	9.50	B	C
ATOM	10330	CH2	TRP	563	87.673	46.980	53.872	1.00	12.48	B	C
ATOM	10331	C	TRP	563	92.880	48.919	57.119	1.00	16.18	B	C
ATOM	10332	O	TRP	563	92.279	48.562	58.132	1.00	15.81	B	O
ATOM	10333	N	ALA	564	93.790	48.161	56.515	1.00	17.44	B	N
ATOM	10334	CA	ALA	564	94.124	46.841	57.042	1.00	17.65	B	C
ATOM	10335	CB	ALA	564	95.216	46.186	56.197	1.00	16.15	B	C
ATOM	10336	C	ALA	564	94.585	46.973	58.489	1.00	18.07	B	C
ATOM	10337	O	ALA	564	94.256	46.127	59.320	1.00	18.92	B	O
ATOM	10338	N	THR	565	95.332	48.037	58.793	1.00	17.73	B	N

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(Continued)

## FIG. 4 - 212

ATOM	10339	CA	THR	565	95.817	48.259	60.159	1.00	17.29	B	C
ATOM	10340	CB	THR	565	96.626	49.551	60.294	1.00	17.13	B	C
ATOM	10341	OG1	THR	565	97.677	49.570	59.330	1.00	20.36	B	O
ATOM	10342	CG2	THR	565	97.238	49.636	61.676	1.00	18.23	B	C
ATOM	10343	C	THR	565	94.665	48.355	61.157	1.00	15.84	B	C
ATOM	10344	O	THR	565	94.738	47.804	62.249	1.00	14.07	B	O
ATOM	10345	N	TYR	566	93.605	49.061	60.781	1.00	15.76	B	N
ATOM	10346	CA	TYR	566	92.455	49.204	61.664	1.00	17.74	B	C
ATOM	10347	CB	TYR	566	91.543	50.335	61.177	1.00	15.61	B	C
ATOM	10348	CG	TYR	566	90.067	50.039	61.311	1.00	17.40	B	C
ATOM	10349	CD1	TYR	566	89.303	49.688	60.195	1.00	17.77	B	C
ATOM	10350	CE1	TYR	566	87.947	49.390	60.310	1.00	15.12	B	C
ATOM	10351	CD2	TYR	566	89.432	50.086	62.556	1.00	18.30	B	C
ATOM	10352	CE2	TYR	566	88.073	49.789	62.682	1.00	17.35	B	C
ATOM	10353	CZ	TYR	566	87.340	49.441	61.550	1.00	17.10	B	C
ATOM	10354	OH	TYR	566	86.005	49.137	61.662	1.00	17.63	B	O
ATOM	10355	C	TYR	566	91.667	47.899	61.777	1.00	19.12	B	C
ATOM	10356	O	TYR	566	91.249	47.517	62.871	1.00	20.12	B	O
ATOM	10357	N	LEU	567	91.481	47.211	60.654	1.00	19.08	B	N
ATOM	10358	CA	LEU	567	90.735	45.959	60.648	1.00	19.66	B	C
ATOM	10359	CB	LEU	567	90.606	45.419	59.223	1.00	18.00	B	C
ATOM	10360	CG	LEU	567	89.728	46.252	58.284	1.00	18.48	B	C
ATOM	10361	CD1	LEU	567	89.735	45.628	56.889	1.00	19.22	B	C
ATOM	10362	CD2	LEU	567	88.310	46.325	58.835	1.00	15.78	B	C
ATOM	10363	C	LEU	567	91.355	44.898	61.544	1.00	20.80	B	C
ATOM	10364	O	LEU	567	90.645	44.102	62.157	1.00	23.88	B	O
ATOM	10365	N	ALA	568	92.677	44.883	61.628	1.00	19.62	B	N
ATOM	10366	CA	ALA	568	93.347	43.898	62.466	1.00	20.08	B	C
ATOM	10367	CB	ALA	568	94.746	43.601	61.907	1.00	18.06	B	C
ATOM	10368	C	ALA	568	93.451	44.362	63.924	1.00	20.52	B	C
ATOM	10369	O	ALA	568	93.319	43.569	64.849	1.00	20.37	B	O
ATOM	10370	N	SER	569	93.674	45.653	64.128	1.00	20.79	B	N
ATOM	10371	CA	SER	569	93.827	46.182	65.474	1.00	21.75	B	C
ATOM	10372	CB	SER	569	94.520	47.545	65.401	1.00	21.85	B	C
ATOM	10373	OG	SER	569	94.546	48.188	66.657	1.00	22.64	B	O
ATOM	10374	C	SER	569	92.525	46.297	66.267	1.00	22.83	B	C
ATOM	10375	O	SER	569	92.505	46.029	67.470	1.00	22.38	B	O
ATOM	10376	N	THR	570	91.444	46.679	65.589	1.00	22.26	B	N
ATOM	10377	CA	THR	570	90.153	46.862	66.232	1.00	21.45	B	C
ATOM	10378	CB	THR	570	89.512	48.191	65.797	1.00	19.91	B	C
ATOM	10379	OG1	THR	570	90.349	49.285	66.188	1.00	21.12	B	O
ATOM	10380	CG2	THR	570	88.143	48.351	66.430	1.00	17.96	B	C
ATOM	10381	C	THR	570	89.132	45.751	65.974	1.00	24.43	B	C
ATOM	10382	O	THR	570	88.453	45.301	66.894	1.00	27.79	B	O
ATOM	10383	N	GLU	571	89.001	45.317	64.727	1.00	23.34	B	N
ATOM	10384	CA	GLU	571	88.030	44.280	64.415	1.00	21.95	B	C
ATOM	10385	CB	GLU	571	87.499	44.481	62.998	1.00	22.83	B	C
ATOM	10386	CG	GLU	571	87.004	45.888	62.709	1.00	24.63	B	C
ATOM	10387	CD	GLU	571	85.957	46.357	63.696	1.00	25.17	B	C

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## FIG. 4 - 213

(Continued)

ATOM	10388	OE1	GLU	571	85.236	45.509	64.258	1.00	28.12	B	O
ATOM	10389	OE2	GLU	571	85.834	47.580	63.897	1.00	26.28	B	O
ATOM	10390	C	GLU	571	88.606	42.874	64.554	1.00	21.35	B	C
ATOM	10391	O	GLU	571	87.903	41.887	64.362	1.00	19.91	B	O
ATOM	10392	N	ASN	572	89.887	42.784	64.894	1.00	22.55	B	N
ATOM	10393	CA	ASN	572	90.539	41.491	65.043	1.00	21.58	B	C
ATOM	10394	CB	ASN	572	89.998	40.744	66.255	1.00	23.76	B	C
ATOM	10395	CG	ASN	572	90.523	41.303	67.552	1.00	27.80	B	C
ATOM	10396	OD1	ASN	572	90.053	42.335	68.035	1.00	30.34	B	O
ATOM	10397	ND2	ASN	572	91.522	40.634	68.121	1.00	30.31	B	N
ATOM	10398	C	ASN	572	90.347	40.639	63.806	1.00	21.12	B	C
ATOM	10399	O	ASN	572	90.112	39.436	63.903	1.00	20.16	B	O
ATOM	10400	N	ILE	573	90.445	41.280	62.645	1.00	19.59	B	N
ATOM	10401	CA	ILE	573	90.311	40.604	61.365	1.00	18.06	B	C
ATOM	10402	CB	ILE	573	89.509	41.456	60.382	1.00	18.14	B	C
ATOM	10403	CG2	ILE	573	89.371	40.735	59.057	1.00	18.53	B	C
ATOM	10404	CG1	ILE	573	88.143	41.778	60.970	1.00	19.49	B	C
ATOM	10405	CD1	ILE	573	87.336	42.735	60.131	1.00	20.04	B	C
ATOM	10406	C	ILE	573	91.706	40.425	60.777	1.00	18.47	B	C
ATOM	10407	O	ILE	573	92.480	41.376	60.739	1.00	19.08	B	O
ATOM	10408	N	ILE	574	92.038	39.216	60.337	1.00	17.57	B	N
ATOM	10409	CA	ILE	574	93.340	38.978	59.724	1.00	18.02	B	C
ATOM	10410	CB	ILE	574	93.724	37.494	59.740	1.00	19.09	B	C
ATOM	10411	CG2	ILE	574	94.950	37.280	58.870	1.00	20.13	B	C
ATOM	10412	CG1	ILE	574	94.004	37.031	61.172	1.00	21.02	B	C
ATOM	10413	CD1	ILE	574	94.330	35.553	61.282	1.00	20.47	B	C
ATOM	10414	C	ILE	574	93.298	39.423	58.265	1.00	17.84	B	C
ATOM	10415	O	ILE	574	92.444	38.981	57.500	1.00	19.48	B	O
ATOM	10416	N	VAL	575	94.217	40.296	57.876	1.00	17.13	B	N
ATOM	10417	CA	VAL	575	94.254	40.777	56.498	1.00	16.42	B	C
ATOM	10418	CB	VAL	575	94.354	42.308	56.430	1.00	16.55	B	C
ATOM	10419	CG1	VAL	575	94.271	42.753	54.985	1.00	16.06	B	C
ATOM	10420	CG2	VAL	575	93.242	42.948	57.261	1.00	15.54	B	C
ATOM	10421	C	VAL	575	95.452	40.187	55.786	1.00	16.02	B	C
ATOM	10422	O	VAL	575	96.592	40.488	56.124	1.00	16.68	B	O
ATOM	10423	N	ALA	576	95.186	39.344	54.797	1.00	16.21	B	N
ATOM	10424	CA	ALA	576	96.246	38.683	54.056	1.00	15.22	B	C
ATOM	10425	CB	ALA	576	96.062	37.176	54.127	1.00	12.38	B	C
ATOM	10426	C	ALA	576	96.330	39.117	52.601	1.00	15.92	B	C
ATOM	10427	O	ALA	576	95.397	39.710	52.046	1.00	16.20	B	O
ATOM	10428	N	SER	577	97.470	38.811	51.996	1.00	14.35	B	N
ATOM	10429	CA	SER	577	97.722	39.123	50.606	1.00	13.57	B	C
ATOM	10430	CB	SER	577	98.368	40.495	50.474	1.00	13.58	B	C
ATOM	10431	OG	SER	577	97.456	41.504	50.866	1.00	16.22	B	O
ATOM	10432	C	SER	577	98.642	38.045	50.069	1.00	13.24	B	C
ATOM	10433	O	SER	577	99.497	37.522	50.788	1.00	13.05	B	O
ATOM	10434	N	PHE	578	98.462	37.712	48.800	1.00	11.98	B	N
ATOM	10435	CA	PHE	578	99.262	36.676	48.183	1.00	11.24	B	C
ATOM	10436	CB	PHE	578	98.418	35.407	48.079	1.00	11.42	B	C

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(Continued)

## FIG. 4 - 214

ATOM	10437	CG	PHE	578	99.136	34.232	47.481	1.00	10.60	B	C
ATOM	10438	CD1	PHE	578	100.196	33.628	48.152	1.00	10.29	B	C
ATOM	10439	CD2	PHE	578	98.697	33.679	46.280	1.00	10.36	B	C
ATOM	10440	CE1	PHE	578	100.805	32.483	47.640	1.00	11.15	B	C
ATOM	10441	CE2	PHE	578	99.297	32.537	45.762	1.00	11.72	B	C
ATOM	10442	CZ	PHE	578	100.354	31.936	46.446	1.00	10.87	B	C
ATOM	10443	C	PHE	578	99.746	37.096	46.805	1.00	10.56	B	C
ATOM	10444	O	PHE	578	99.002	37.704	46.039	1.00	10.76	B	O
ATOM	10445	N	ASP	579	101.005	36.780	46.516	1.00	11.14	B	N
ATOM	10446	CA	ASP	579	101.617	37.069	45.227	1.00	9.94	B	C
ATOM	10447	CB	ASP	579	103.008	37.682	45.401	1.00	9.15	B	C
ATOM	10448	CG	ASP	579	102.957	39.090	45.954	1.00	13.00	B	C
ATOM	10449	OD1	ASP	579	102.053	39.842	45.532	1.00	14.87	B	O
ATOM	10450	OD2	ASP	579	103.816	39.451	46.796	1.00	11.19	B	O
ATOM	10451	C	ASP	579	101.734	35.741	44.488	1.00	11.60	B	C
ATOM	10452	O	ASP	579	102.633	34.927	44.753	1.00	12.07	B	O
ATOM	10453	N	GLY	580	100.809	35.510	43.570	1.00	10.77	B	N
ATOM	10454	CA	GLY	580	100.838	34.274	42.815	1.00	11.96	B	C
ATOM	10455	C	GLY	580	101.458	34.470	41.450	1.00	13.34	B	C
ATOM	10456	O	GLY	580	102.269	35.376	41.227	1.00	12.96	B	O
ATOM	10457	N	ARG	581	101.080	33.611	40.521	1.00	14.18	B	N
ATOM	10458	CA	ARG	581	101.615	33.714	39.187	1.00	15.34	B	C
ATOM	10459	CB	ARG	581	101.085	32.570	38.338	1.00	13.67	B	C
ATOM	10460	CG	ARG	581	101.809	31.283	38.666	1.00	15.30	B	C
ATOM	10461	CD	ARG	581	101.172	30.076	38.023	1.00	14.62	B	C
ATOM	10462	NE	ARG	581	99.980	29.652	38.740	1.00	13.01	B	N
ATOM	10463	CZ	ARG	581	99.186	28.672	38.330	1.00	13.69	B	C
ATOM	10464	NH1	ARG	581	99.467	28.024	37.207	1.00	13.99	B	N
ATOM	10465	NH2	ARG	581	98.112	28.348	39.036	1.00	12.41	B	N
ATOM	10466	C	ARG	581	101.237	35.069	38.624	1.00	17.21	B	C
ATOM	10467	O	ARG	581	100.175	35.615	38.934	1.00	17.96	B	O
ATOM	10468	N	GLY	582	102.128	35.628	37.817	1.00	18.14	B	N
ATOM	10469	CA	GLY	582	101.868	36.933	37.258	1.00	17.73	B	C
ATOM	10470	C	GLY	582	102.454	37.998	38.159	1.00	16.81	B	C
ATOM	10471	O	GLY	582	102.557	39.151	37.754	1.00	18.98	B	O
ATOM	10472	N	SER	583	102.835	37.625	39.378	1.00	15.90	B	N
ATOM	10473	CA	SER	583	103.423	38.588	40.309	1.00	16.60	B	C
ATOM	10474	CB	SER	583	103.437	38.024	41.730	1.00	17.47	B	C
ATOM	10475	OG	SER	583	104.229	36.856	41.811	1.00	21.54	B	O
ATOM	10476	C	SER	583	104.841	38.901	39.841	1.00	15.56	B	C
ATOM	10477	O	SER	583	105.389	38.176	39.013	1.00	17.79	B	O
ATOM	10478	N	GLY	584	105.441	39.970	40.359	1.00	14.64	B	N
ATOM	10479	CA	GLY	584	106.776	40.334	39.908	1.00	13.05	B	C
ATOM	10480	C	GLY	584	107.969	40.158	40.831	1.00	12.28	B	C
ATOM	10481	O	GLY	584	107.851	39.648	41.949	1.00	11.78	B	O
ATOM	10482	N	TYR	585	109.129	40.583	40.325	1.00	12.34	B	N
ATOM	10483	CA	TYR	585	110.412	40.536	41.034	1.00	12.19	B	C
ATOM	10484	CB	TYR	585	110.335	41.383	42.304	1.00	11.93	B	C
ATOM	10485	CG	TYR	585	109.704	42.719	42.047	1.00	12.41	B	C

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## FIG. 4 - 215

(Continued)

ATOM	10486	CD1	TYR	585	110.370	43.694	41.297	1.00	12.30	B	C
ATOM	10487	CE1	TYR	585	109.756	44.891	40.979	1.00	12.43	B	C
ATOM	10488	CD2	TYR	585	108.408	42.983	42.478	1.00	10.95	B	C
ATOM	10489	CE2	TYR	585	107.783	44.179	42.167	1.00	12.28	B	C
ATOM	10490	CZ	TYR	585	108.459	45.126	41.418	1.00	13.31	B	C
ATOM	10491	OH	TYR	585	107.831	46.306	41.109	1.00	14.33	B	O
ATOM	10492	C	TYR	585	110.883	39.141	41.394	1.00	12.01	B	C
ATOM	10493	O	TYR	585	111.673	38.979	42.319	1.00	13.01	B	O
ATOM	10494	N	GLN	586	110.413	38.144	40.655	1.00	11.45	B	N
ATOM	10495	CA	GLN	586	110.787	36.763	40.906	1.00	11.62	B	C
ATOM	10496	CB	GLN	586	109.639	36.071	41.641	1.00	10.30	B	C
ATOM	10497	CG	GLN	586	109.178	36.854	42.867	1.00	14.38	B	C
ATOM	10498	CD	GLN	586	107.749	36.533	43.295	1.00	15.38	B	C
ATOM	10499	OE1	GLN	586	107.468	35.452	43.816	1.00	12.14	B	O
ATOM	10500	NE2	GLN	586	106.835	37.478	43.060	1.00	15.36	B	N
ATOM	10501	C	GLN	586	111.118	36.023	39.602	1.00	12.85	B	C
ATOM	10502	O	GLN	586	111.173	34.786	39.574	1.00	13.97	B	O
ATOM	10503	N	GLY	587	111.336	36.778	38.525	1.00	11.70	B	N
ATOM	10504	CA	GLY	587	111.641	36.168	37.242	1.00	11.61	B	C
ATOM	10505	C	GLY	587	110.405	35.960	36.373	1.00	14.10	B	C
ATOM	10506	O	GLY	587	109.302	35.786	36.884	1.00	13.91	B	O
ATOM	10507	N	ASP	588	110.595	35.949	35.054	1.00	16.19	B	N
ATOM	10508	CA	ASP	588	109.500	35.776	34.105	1.00	17.70	B	C
ATOM	10509	CB	ASP	588	110.002	35.993	32.680	1.00	18.98	B	C
ATOM	10510	CG	ASP	588	110.708	37.312	32.505	1.00	20.57	B	C
ATOM	10511	OD1	ASP	588	110.236	38.335	33.040	1.00	23.28	B	O
ATOM	10512	OD2	ASP	588	111.738	37.327	31.809	1.00	23.25	B	O
ATOM	10513	C	ASP	588	108.723	34.454	34.139	1.00	17.46	B	C
ATOM	10514	O	ASP	588	107.608	34.389	33.635	1.00	16.74	B	O
ATOM	10515	N	LYS	589	109.294	33.397	34.697	1.00	18.02	B	N
ATOM	10516	CA	LYS	589	108.559	32.143	34.734	1.00	20.00	B	C
ATOM	10517	CB	LYS	589	109.383	31.030	35.372	1.00	22.21	B	C
ATOM	10518	CG	LYS	589	108.633	29.710	35.443	1.00	27.16	B	C
ATOM	10519	CD	LYS	589	109.526	28.579	35.940	1.00	32.47	B	C
ATOM	10520	CE	LYS	589	108.753	27.273	36.111	1.00	33.79	B	C
ATOM	10521	NZ	LYS	589	109.605	26.232	36.771	1.00	35.98	B	N
ATOM	10522	C	LYS	589	107.290	32.362	35.536	1.00	20.94	B	C
ATOM	10523	O	LYS	589	106.244	31.781	35.242	1.00	23.79	B	O
ATOM	10524	N	ILE	590	107.384	33.212	36.552	1.00	18.06	B	N
ATOM	10525	CA	ILE	590	106.237	33.523	37.379	1.00	14.07	B	C
ATOM	10526	CB	ILE	590	106.681	33.901	38.814	1.00	11.33	B	C
ATOM	10527	CG2	ILE	590	105.585	34.654	39.538	1.00	9.61	B	C
ATOM	10528	CG1	ILE	590	107.057	32.635	39.585	1.00	10.89	B	C
ATOM	10529	CD1	ILE	590	107.750	32.888	40.897	1.00	7.05	B	C
ATOM	10530	C	ILE	590	105.461	34.682	36.753	1.00	15.70	B	C
ATOM	10531	O	ILE	590	104.254	34.583	36.511	1.00	16.31	B	O
ATOM	10532	N	MET	591	106.159	35.774	36.465	1.00	15.00	B	N
ATOM	10533	CA	MET	591	105.506	36.948	35.907	1.00	14.79	B	C
ATOM	10534	CB	MET	591	106.512	38.088	35.759	1.00	14.22	B	C

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## FIG. 4 - 216

(Continued)

ATOM	10535	CG	MET	591	105.854	39.452	35.581	1.00	18.55	B	C
ATOM	10536	SD	MET	591	107.027	40.830	35.526	1.00	17.84	B	S
ATOM	10537	CE	MET	591	107.813	40.502	33.933	1.00	16.39	B	C
ATOM	10538	C	MET	591	104.788	36.699	34.582	1.00	14.86	B	C
ATOM	10539	O	MET	591	103.643	37.113	34.418	1.00	14.45	B	O
ATOM	10540	N	HIS	592	105.451	36.022	33.647	1.00	14.66	B	N
ATOM	10541	CA	HIS	592	104.863	35.725	32.343	1.00	14.33	B	C
ATOM	10542	CB	HIS	592	105.962	35.424	31.332	1.00	15.14	B	C
ATOM	10543	CG	HIS	592	106.753	36.626	30.922	1.00	17.56	B	C
ATOM	10544	CD2	HIS	592	106.626	37.933	31.252	1.00	17.20	B	C
ATOM	10545	ND1	HIS	592	107.810	36.555	30.041	1.00	17.84	B	N
ATOM	10546	CE1	HIS	592	108.300	37.765	29.845	1.00	16.59	B	C
ATOM	10547	NE2	HIS	592	107.598	38.620	30.567	1.00	16.88	B	N
ATOM	10548	C	HIS	592	103.859	34.569	32.355	1.00	15.17	B	C
ATOM	10549	O	HIS	592	103.224	34.274	31.344	1.00	15.89	B	O
ATOM	10550	N	ALA	593	103.708	33.917	33.500	1.00	15.86	B	N
ATOM	10551	CA	ALA	593	102.775	32.810	33.615	1.00	14.02	B	C
ATOM	10552	CB	ALA	593	102.690	32.353	35.060	1.00	13.60	B	C
ATOM	10553	C	ALA	593	101.393	33.195	33.106	1.00	15.66	B	C
ATOM	10554	O	ALA	593	100.647	32.335	32.631	1.00	17.83	B	O
ATOM	10555	N	ILE	594	101.043	34.478	33.207	1.00	16.63	B	N
ATOM	10556	CA	ILE	594	99.731	34.945	32.745	1.00	16.87	B	C
ATOM	10557	CB	ILE	594	99.035	35.857	33.791	1.00	15.87	B	C
ATOM	10558	CG2	ILE	594	98.506	35.017	34.932	1.00	16.36	B	C
ATOM	10559	CG1	ILE	594	100.006	36.915	34.321	1.00	16.86	B	C
ATOM	10560	CD1	ILE	594	100.533	37.882	33.274	1.00	16.67	B	C
ATOM	10561	C	ILE	594	99.748	35.689	31.413	1.00	17.96	B	C
ATOM	10562	O	ILE	594	98.884	36.525	31.160	1.00	19.03	B	O
ATOM	10563	N	ASN	595	100.718	35.385	30.558	1.00	17.93	B	N
ATOM	10564	CA	ASN	595	100.802	36.050	29.263	1.00	19.09	B	C
ATOM	10565	CB	ASN	595	102.140	35.737	28.592	1.00	19.22	B	C
ATOM	10566	CG	ASN	595	102.291	36.441	27.260	1.00	19.91	B	C
ATOM	10567	OD1	ASN	595	102.320	37.668	27.198	1.00	19.01	B	O
ATOM	10568	ND2	ASN	595	102.377	35.667	26.184	1.00	19.95	B	N
ATOM	10569	C	ASN	595	99.659	35.641	28.330	1.00	19.09	B	C
ATOM	10570	O	ASN	595	99.456	34.460	28.076	1.00	19.31	B	O
ATOM	10571	N	ARG	596	98.933	36.630	27.814	1.00	19.66	B	N
ATOM	10572	CA	ARG	596	97.799	36.406	26.911	1.00	20.07	B	C
ATOM	10573	CB	ARG	596	98.212	35.588	25.677	1.00	17.78	B	C
ATOM	10574	CG	ARG	596	99.233	36.247	24.756	1.00	17.26	B	C
ATOM	10575	CD	ARG	596	99.655	35.296	23.636	1.00	17.14	B	C
ATOM	10576	NE	ARG	596	98.553	34.982	22.728	1.00	17.97	B	N
ATOM	10577	CZ	ARG	596	98.102	35.816	21.795	1.00	19.85	B	C
ATOM	10578	NH1	ARG	596	98.671	37.005	21.640	1.00	21.47	B	N
ATOM	10579	NH2	ARG	596	97.060	35.486	21.045	1.00	18.12	B	N
ATOM	10580	C	ARG	596	96.692	35.655	27.632	1.00	21.03	B	C
ATOM	10581	O	ARG	596	95.731	35.213	27.005	1.00	22.67	B	O
ATOM	10582	N	ARG	597	96.811	35.529	28.948	1.00	20.90	B	N
ATOM	10583	CA	ARG	597	95.831	34.770	29.714	1.00	20.85	B	C

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(Continued)

## FIG. 4 - 217

ATOM	10584	CB	ARG	597	96.437	33.414	30.078	1.00	23.88	B	C
ATOM	10585	CG	ARG	597	95.850	32.257	29.300	1.00	31.40	B	C
ATOM	10586	CD	ARG	597	95.913	32.520	27.810	1.00	34.67	B	C
ATOM	10587	NE	ARG	597	95.006	31.660	27.059	1.00	35.49	B	N
ATOM	10588	CZ	ARG	597	94.776	31.792	25.759	1.00	35.98	B	C
ATOM	10589	NH1	ARG	597	95.386	32.748	25.075	1.00	35.20	B	N
ATOM	10590	NH2	ARG	597	93.933	30.974	25.145	1.00	39.12	B	N
ATOM	10591	C	ARG	597	95.292	35.429	30.976	1.00	18.83	B	C
ATOM	10592	O	ARG	597	94.981	34.739	31.945	1.00	17.54	B	O
ATOM	10593	N	LEU	598	95.175	36.751	30.964	1.00	16.66	B	N
ATOM	10594	CA	LEU	598	94.678	37.477	32.125	1.00	15.71	B	C
ATOM	10595	CB	LEU	598	94.482	38.959	31.769	1.00	12.95	B	C
ATOM	10596	CG	LEU	598	95.523	39.990	32.248	1.00	12.69	B	C
ATOM	10597	CD1	LEU	598	96.939	39.473	32.106	1.00	11.40	B	C
ATOM	10598	CD2	LEU	598	95.361	41.267	31.466	1.00	9.68	B	C
ATOM	10599	C	LEU	598	93.369	36.870	32.642	1.00	17.19	B	C
ATOM	10600	O	LEU	598	92.533	36.398	31.863	1.00	17.25	B	O
ATOM	10601	N	GLY	599	93.207	36.864	33.961	1.00	16.06	B	N
ATOM	10602	CA	GLY	599	91.997	36.328	34.547	1.00	16.44	B	C
ATOM	10603	C	GLY	599	91.987	34.824	34.735	1.00	17.37	B	C
ATOM	10604	O	GLY	599	90.921	34.221	34.843	1.00	17.28	B	O
ATOM	10605	N	THR	600	93.164	34.213	34.786	1.00	17.73	B	N
ATOM	10606	CA	THR	600	93.247	32.775	34.972	1.00	17.95	B	C
ATOM	10607	CB	THR	600	93.823	32.091	33.722	1.00	18.93	B	C
ATOM	10608	OG1	THR	600	95.185	32.495	33.530	1.00	17.74	B	O
ATOM	10609	CG2	THR	600	93.000	32.463	32.491	1.00	17.48	B	C
ATOM	10610	C	THR	600	94.087	32.384	36.183	1.00	19.93	B	C
ATOM	10611	O	THR	600	93.574	32.285	37.295	1.00	21.69	B	O
ATOM	10612	N	PHE	601	95.382	32.177	35.971	1.00	21.11	B	N
ATOM	10613	CA	PHE	601	96.279	31.768	37.048	1.00	21.56	B	C
ATOM	10614	CB	PHE	601	97.686	31.542	36.494	1.00	20.77	B	C
ATOM	10615	CG	PHE	601	97.757	30.452	35.475	1.00	21.75	B	C
ATOM	10616	CD1	PHE	601	98.676	30.513	34.439	1.00	23.50	B	C
ATOM	10617	CD2	PHE	601	96.896	29.366	35.539	1.00	21.83	B	C
ATOM	10618	CE1	PHE	601	98.731	29.502	33.474	1.00	24.75	B	C
ATOM	10619	CE2	PHE	601	96.949	28.356	34.581	1.00	22.61	B	C
ATOM	10620	CZ	PHE	601	97.868	28.427	33.547	1.00	20.03	B	C
ATOM	10621	C	PHE	601	96.346	32.710	38.244	1.00	21.61	B	C
ATOM	10622	O	PHE	601	96.437	32.247	39.386	1.00	23.03	B	O
ATOM	10623	N	GLU	602	96.312	34.018	37.997	1.00	20.14	B	N
ATOM	10624	CA	GLU	602	96.374	34.976	39.097	1.00	19.30	B	C
ATOM	10625	CB	GLU	602	96.505	36.422	38.581	1.00	16.90	B	C
ATOM	10626	CG	GLU	602	95.193	37.072	38.135	1.00	17.16	B	C
ATOM	10627	CD	GLU	602	94.857	36.847	36.661	1.00	17.31	B	C
ATOM	10628	OE1	GLU	602	94.930	35.696	36.184	1.00	18.92	B	O
ATOM	10629	OE2	GLU	602	94.505	37.830	35.981	1.00	16.38	B	O
ATOM	10630	C	GLU	602	95.111	34.838	39.952	1.00	18.97	B	C
ATOM	10631	O	GLU	602	95.170	34.953	41.179	1.00	18.54	B	O
ATOM	10632	N	VAL	603	93.979	34.584	39.296	1.00	19.02	B	N

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(Continued)

## FIG. 4 - 218

ATOM	10633	CA	VAL	603	92.696	34.413	39.984	1.00	21.62	B	C
ATOM	10634	CB	VAL	603	91.513	34.471	38.999	1.00	21.51	B	C
ATOM	10635	CG1	VAL	603	90.233	34.055	39.701	1.00	19.24	B	C
ATOM	10636	CG2	VAL	603	91.380	35.876	38.442	1.00	21.00	B	C
ATOM	10637	C	VAL	603	92.643	33.073	40.716	1.00	22.35	B	C
ATOM	10638	O	VAL	603	92.160	32.989	41.848	1.00	21.06	B	O
ATOM	10639	N	GLU	604	93.141	32.031	40.059	1.00	22.98	B	N
ATOM	10640	CA	GLU	604	93.182	30.702	40.656	1.00	26.04	B	C
ATOM	10641	CB	GLU	604	93.721	29.681	39.645	1.00	28.46	B	C
ATOM	10642	CG	GLU	604	92.956	29.671	38.326	1.00	35.94	B	C
ATOM	10643	CD	GLU	604	93.559	28.742	37.273	1.00	40.17	B	C
ATOM	10644	OE1	GLU	604	93.215	28.911	36.076	1.00	40.47	B	O
ATOM	10645	OE2	GLU	604	94.360	27.844	37.637	1.00	41.61	B	O
ATOM	10646	C	GLU	604	94.072	30.705	41.905	1.00	24.63	B	C
ATOM	10647	O	GLU	604	93.657	30.255	42.976	1.00	25.47	B	O
ATOM	10648	N	ASP	605	95.286	31.234	41.775	1.00	22.17	B	N
ATOM	10649	CA	ASP	605	96.213	31.255	42.900	1.00	21.12	B	C
ATOM	10650	CB	ASP	605	97.568	31.827	42.463	1.00	23.09	B	C
ATOM	10651	CG	ASP	605	98.263	30.958	41.414	1.00	24.43	B	C
ATOM	10652	OD1	ASP	605	97.894	29.774	41.266	1.00	26.59	B	O
ATOM	10653	OD2	ASP	605	99.188	31.453	40.742	1.00	25.60	B	O
ATOM	10654	C	ASP	605	95.712	31.967	44.159	1.00	19.42	B	C
ATOM	10655	O	ASP	605	96.099	31.598	45.260	1.00	19.67	B	O
ATOM	10656	N	GLN	606	94.868	32.983	44.014	1.00	17.23	B	N
ATOM	10657	CA	GLN	606	94.337	33.673	45.192	1.00	16.41	B	C
ATOM	10658	CB	GLN	606	93.576	34.951	44.795	1.00	17.09	B	C
ATOM	10659	CG	GLN	606	94.407	36.070	44.165	1.00	15.81	B	C
ATOM	10660	CD	GLN	606	95.332	36.748	45.162	1.00	15.36	B	C
ATOM	10661	OE1	GLN	606	94.879	37.283	46.173	1.00	13.19	B	O
ATOM	10662	NE2	GLN	606	96.637	36.730	44.878	1.00	14.39	B	N
ATOM	10663	C	GLN	606	93.360	32.706	45.878	1.00	15.71	B	C
ATOM	10664	O	GLN	606	93.337	32.583	47.102	1.00	14.30	B	O
ATOM	10665	N	ILE	607	92.549	32.030	45.070	1.00	13.95	B	N
ATOM	10666	CA	ILE	607	91.584	31.076	45.583	1.00	13.95	B	C
ATOM	10667	CB	ILE	607	90.772	30.437	44.448	1.00	12.90	B	C
ATOM	10668	CG2	ILE	607	89.925	29.294	44.996	1.00	11.78	B	C
ATOM	10669	CG1	ILE	607	89.909	31.504	43.773	1.00	12.90	B	C
ATOM	10670	CD1	ILE	607	89.162	31.016	42.560	1.00	11.00	B	C
ATOM	10671	C	ILE	607	92.330	29.985	46.318	1.00	15.04	B	C
ATOM	10672	O	ILE	607	92.008	29.670	47.462	1.00	15.40	B	O
ATOM	10673	N	GLU	608	93.331	29.413	45.652	1.00	16.29	B	N
ATOM	10674	CA	GLU	608	94.144	28.359	46.246	1.00	18.48	B	C
ATOM	10675	CB	GLU	608	95.180	27.864	45.235	1.00	18.74	B	C
ATOM	10676	CG	GLU	608	96.164	26.851	45.792	1.00	22.43	B	C
ATOM	10677	CD	GLU	608	95.498	25.557	46.213	1.00	29.00	B	C
ATOM	10678	OE1	GLU	608	96.096	24.817	47.032	1.00	32.52	B	O
ATOM	10679	OE2	GLU	608	94.382	25.274	45.721	1.00	31.62	B	O
ATOM	10680	C	GLU	608	94.848	28.889	47.501	1.00	20.58	B	C
ATOM	10681	O	GLU	608	95.114	28.138	48.446	1.00	23.01	B	O

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## FIG. 4 - 219

(Continued)

ATOM	10682	N	ALA	609	95.150	30.183	47.506	1.00	19.99	B	N
ATOM	10683	CA	ALA	609	95.811	30.789	48.646	1.00	21.28	B	C
ATOM	10684	CB	ALA	609	96.269	32.196	48.310	1.00	19.81	B	C
ATOM	10685	C	ALA	609	94.826	30.819	49.797	1.00	21.63	B	C
ATOM	10686	O	ALA	609	95.152	30.426	50.915	1.00	21.88	B	O
ATOM	10687	N	ALA	610	93.618	31.286	49.516	1.00	23.07	B	N
ATOM	10688	CA	ALA	610	92.580	31.358	50.535	1.00	25.56	B	C
ATOM	10689	CB	ALA	610	91.317	31.963	49.957	1.00	25.38	B	C
ATOM	10690	C	ALA	610	92.300	29.952	51.024	1.00	26.13	B	C
ATOM	10691	O	ALA	610	92.256	29.694	52.223	1.00	25.97	B	O
ATOM	10692	N	ARG	611	92.119	29.044	50.073	1.00	28.12	B	N
ATOM	10693	CA	ARG	611	91.838	27.647	50.374	1.00	28.88	B	C
ATOM	10694	CB	ARG	611	91.886	26.826	49.087	1.00	27.27	B	C
ATOM	10695	CG	ARG	611	91.518	25.372	49.260	1.00	28.40	B	C
ATOM	10696	CD	ARG	611	91.547	24.668	47.925	1.00	30.54	B	C
ATOM	10697	NE	ARG	611	90.501	25.152	47.028	1.00	33.73	B	N
ATOM	10698	CZ	ARG	611	90.628	25.223	45.706	1.00	36.39	B	C
ATOM	10699	NH1	ARG	611	91.764	24.848	45.129	1.00	38.00	B	N
ATOM	10700	NH2	ARG	611	89.615	25.645	44.956	1.00	37.15	B	N
ATOM	10701	C	ARG	611	92.826	27.082	51.391	1.00	29.24	B	C
ATOM	10702	O	ARG	611	92.446	26.330	52.287	1.00	30.51	B	O
ATOM	10703	N	GLN	612	94.092	27.452	51.260	1.00	30.24	B	N
ATOM	10704	CA	GLN	612	95.105	26.965	52.182	1.00	30.75	B	C
ATOM	10705	CB	GLN	612	96.491	27.029	51.532	1.00	29.62	B	C
ATOM	10706	CG	GLN	612	96.738	25.866	50.581	1.00	31.27	B	C
ATOM	10707	CD	GLN	612	98.183	25.741	50.150	1.00	32.19	B	C
ATOM	10708	OE1	GLN	612	99.097	25.778	50.979	1.00	32.20	B	O
ATOM	10709	NE2	GLN	612	98.400	25.578	48.848	1.00	31.86	B	N
ATOM	10710	C	GLN	612	95.109	27.691	53.524	1.00	31.36	B	C
ATOM	10711	O	GLN	612	95.441	27.095	54.545	1.00	32.39	B	O
ATOM	10712	N	PHE	613	94.740	28.969	53.533	1.00	31.39	B	N
ATOM	10713	CA	PHE	613	94.705	29.717	54.784	1.00	30.50	B	C
ATOM	10714	CB	PHE	613	94.527	31.217	54.538	1.00	30.43	B	C
ATOM	10715	CG	PHE	613	95.651	31.853	53.775	1.00	31.06	B	C
ATOM	10716	CD1	PHE	613	96.974	31.532	54.058	1.00	32.48	B	C
ATOM	10717	CD2	PHE	613	95.385	32.805	52.796	1.00	30.25	B	C
ATOM	10718	CE1	PHE	613	98.024	32.156	53.371	1.00	32.97	B	C
ATOM	10719	CE2	PHE	613	96.419	33.432	52.109	1.00	31.17	B	C
ATOM	10720	CZ	PHE	613	97.742	33.109	52.394	1.00	32.13	B	C
ATOM	10721	C	PHE	613	93.531	29.214	55.607	1.00	30.36	B	C
ATOM	10722	O	PHE	613	93.572	29.216	56.830	1.00	28.96	B	O
ATOM	10723	N	SER	614	92.478	28.786	54.923	1.00	31.88	B	N
ATOM	10724	CA	SER	614	91.292	28.286	55.600	1.00	34.43	B	C
ATOM	10725	CB	SER	614	90.141	28.104	54.607	1.00	34.30	B	C
ATOM	10726	OG	SER	614	90.419	27.055	53.697	1.00	34.39	B	O
ATOM	10727	C	SER	614	91.609	26.953	56.264	1.00	35.74	B	C
ATOM	10728	O	SER	614	90.908	26.519	57.178	1.00	37.21	B	O
ATOM	10729	N	LYS	615	92.670	26.307	55.797	1.00	36.52	B	N
ATOM	10730	CA	LYS	615	93.079	25.030	56.350	1.00	37.25	B	C

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(Continued)

## FIG. 4 - 220

ATOM	10731	CB	LYS	615	93.781	24.196	55.283	1.00	37.94	B	C
ATOM	10732	CG	LYS	615	92.839	23.516	54.293	1.00	40.25	B	C
ATOM	10733	CD	LYS	615	93.595	23.050	53.053	1.00	42.18	B	C
ATOM	10734	CE	LYS	615	94.883	22.317	53.419	1.00	42.76	B	C
ATOM	10735	NZ	LYS	615	95.776	22.147	52.237	1.00	43.07	B	N
ATOM	10736	C	LYS	615	94.001	25.231	57.544	1.00	37.98	B	C
ATOM	10737	O	LYS	615	94.379	24.275	58.217	1.00	40.67	B	O
ATOM	10738	N	MET	616	94.373	26.474	57.809	1.00	37.04	B	N
ATOM	10739	CA	MET	616	95.240	26.744	58.948	1.00	36.91	B	C
ATOM	10740	CB	MET	616	96.021	28.047	58.738	1.00	36.80	B	C
ATOM	10741	CG	MET	616	97.042	27.961	57.613	1.00	36.28	B	C
ATOM	10742	SD	MET	616	97.847	29.532	57.282	1.00	40.04	B	S
ATOM	10743	CE	MET	616	99.135	29.023	56.125	1.00	35.34	B	C
ATOM	10744	C	MET	616	94.370	26.817	60.200	1.00	35.92	B	C
ATOM	10745	O	MET	616	93.181	27.143	60.130	1.00	35.52	B	O
ATOM	10746	N	GLY	617	94.973	26.514	61.343	1.00	33.40	B	N
ATOM	10747	CA	GLY	617	94.233	26.505	62.587	1.00	31.05	B	C
ATOM	10748	C	GLY	617	93.584	27.783	63.072	1.00	29.42	B	C
ATOM	10749	O	GLY	617	92.516	27.729	63.689	1.00	30.60	B	O
ATOM	10750	N	PHE	618	94.202	28.926	62.797	1.00	26.74	B	N
ATOM	10751	CA	PHE	618	93.676	30.204	63.271	1.00	25.54	B	C
ATOM	10752	CB	PHE	618	94.852	31.118	63.636	1.00	26.06	B	C
ATOM	10753	CG	PHE	618	95.898	31.216	62.563	1.00	25.52	B	C
ATOM	10754	CD1	PHE	618	95.763	32.127	61.523	1.00	25.78	B	C
ATOM	10755	CD2	PHE	618	97.012	30.385	62.588	1.00	25.30	B	C
ATOM	10756	CE1	PHE	618	96.726	32.214	60.518	1.00	26.10	B	C
ATOM	10757	CE2	PHE	618	97.981	30.459	61.590	1.00	26.94	B	C
ATOM	10758	CZ	PHE	618	97.836	31.380	60.549	1.00	27.08	B	C
ATOM	10759	C	PHE	618	92.706	30.948	62.353	1.00	24.88	B	C
ATOM	10760	O	PHE	618	92.319	32.079	62.644	1.00	24.17	B	O
ATOM	10761	N	VAL	619	92.297	30.313	61.259	1.00	24.78	B	N
ATOM	10762	CA	VAL	619	91.381	30.947	60.324	1.00	25.04	B	C
ATOM	10763	CB	VAL	619	91.913	30.876	58.875	1.00	25.17	B	C
ATOM	10764	CG1	VAL	619	91.007	31.665	57.945	1.00	23.09	B	C
ATOM	10765	CG2	VAL	619	93.326	31.415	58.817	1.00	26.33	B	C
ATOM	10766	C	VAL	619	90.004	30.303	60.371	1.00	25.53	B	C
ATOM	10767	O	VAL	619	89.873	29.083	60.378	1.00	25.84	B	O
ATOM	10768	N	ASP	620	88.981	31.146	60.405	1.00	26.00	B	N
ATOM	10769	CA	ASP	620	87.601	30.701	60.449	1.00	26.41	B	C
ATOM	10770	CB	ASP	620	86.779	31.717	61.238	1.00	26.64	B	C
ATOM	10771	CG	ASP	620	85.324	31.334	61.355	1.00	27.36	B	C
ATOM	10772	OD1	ASP	620	84.591	32.074	62.041	1.00	27.95	B	O
ATOM	10773	OD2	ASP	620	84.914	30.306	60.765	1.00	26.86	B	O
ATOM	10774	C	ASP	620	87.104	30.610	59.011	1.00	27.59	B	C
ATOM	10775	O	ASP	620	86.687	31.610	58.435	1.00	27.47	B	O
ATOM	10776	N	ASN	621	87.144	29.409	58.438	1.00	29.06	B	N
ATOM	10777	CA	ASN	621	86.733	29.213	57.053	1.00	30.04	B	C
ATOM	10778	CB	ASN	621	86.925	27.752	56.622	1.00	33.33	B	C
ATOM	10779	CG	ASN	621	86.022	26.782	57.377	1.00	36.94	B	C

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## FIG. 4 - 2 2 1

(Continued)

ATOM	10780	OD1	ASN	621	84.795	26.940	57.415	1.00	38.23	B	O
ATOM	10781	ND2	ASN	621	86.630	25.763	57.972	1.00	39.37	B	N
ATOM	10782	C	ASN	621	85.310	29.639	56.756	1.00	29.63	B	C
ATOM	10783	O	ASN	621	84.887	29.626	55.604	1.00	30.93	B	O
ATOM	10784	N	LYS	622	84.563	30.007	57.787	1.00	28.32	B	N
ATOM	10785	CA	LYS	622	83.195	30.441	57.573	1.00	27.00	B	C
ATOM	10786	CB	LYS	622	82.303	29.986	58.740	1.00	29.24	B	C
ATOM	10787	CG	LYS	622	82.062	28.471	58.738	1.00	32.47	B	C
ATOM	10788	CD	LYS	622	81.029	28.002	59.761	1.00	33.84	B	C
ATOM	10789	CE	LYS	622	81.527	28.099	61.197	1.00	35.48	B	C
ATOM	10790	NZ	LYS	622	81.571	29.501	61.703	1.00	36.73	B	N
ATOM	10791	C	LYS	622	83.168	31.957	57.404	1.00	25.42	B	C
ATOM	10792	O	LYS	622	82.145	32.543	57.047	1.00	26.19	B	O
ATOM	10793	N	ARG	623	84.314	32.583	57.642	1.00	21.83	B	N
ATOM	10794	CA	ARG	623	84.436	34.023	57.515	1.00	18.89	B	C
ATOM	10795	CB	ARG	623	84.380	34.664	58.895	1.00	17.53	B	C
ATOM	10796	CG	ARG	623	83.019	34.573	59.510	1.00	16.79	B	C
ATOM	10797	CD	ARG	623	83.122	34.394	60.991	1.00	19.29	B	C
ATOM	10798	NE	ARG	623	83.405	35.632	61.690	1.00	19.11	B	N
ATOM	10799	CZ	ARG	623	84.207	35.718	62.743	1.00	18.68	B	C
ATOM	10800	NH1	ARG	623	84.812	34.639	63.212	1.00	16.76	B	N
ATOM	10801	NH2	ARG	623	84.388	36.884	63.336	1.00	22.60	B	N
ATOM	10802	C	ARG	623	85.711	34.440	56.792	1.00	18.21	B	C
ATOM	10803	O	ARG	623	86.719	34.776	57.414	1.00	19.54	B	O
ATOM	10804	N	ILE	624	85.651	34.412	55.468	1.00	16.09	B	N
ATOM	10805	CA	ILE	624	86.769	34.798	54.629	1.00	16.59	B	C
ATOM	10806	CB	ILE	624	87.439	33.572	53.991	1.00	18.45	B	C
ATOM	10807	CG2	ILE	624	88.563	34.017	53.059	1.00	18.66	B	C
ATOM	10808	CG1	ILE	624	87.971	32.647	55.088	1.00	19.91	B	C
ATOM	10809	CD1	ILE	624	88.623	31.385	54.564	1.00	22.12	B	C
ATOM	10810	C	ILE	624	86.230	35.695	53.519	1.00	16.74	B	C
ATOM	10811	O	ILE	624	85.402	35.268	52.710	1.00	17.92	B	O
ATOM	10812	N	ALA	625	86.688	36.939	53.494	1.00	15.06	B	N
ATOM	10813	CA	ALA	625	86.250	37.886	52.488	1.00	15.59	B	C
ATOM	10814	CB	ALA	625	85.816	39.174	53.155	1.00	18.31	B	C
ATOM	10815	C	ALA	625	87.375	38.159	51.503	1.00	16.90	B	C
ATOM	10816	O	ALA	625	88.431	37.523	51.558	1.00	16.49	B	O
ATOM	10817	N	ILE	626	87.149	39.107	50.598	1.00	16.75	B	N
ATOM	10818	CA	ILE	626	88.158	39.454	49.608	1.00	17.73	B	C
ATOM	10819	CB	ILE	626	88.207	38.397	48.478	1.00	19.21	B	C
ATOM	10820	CG2	ILE	626	86.883	38.365	47.742	1.00	19.01	B	C
ATOM	10821	CG1	ILE	626	89.348	38.713	47.511	1.00	18.94	B	C
ATOM	10822	CD1	ILE	626	89.576	37.642	46.471	1.00	20.78	B	C
ATOM	10823	C	ILE	626	87.850	40.810	49.003	1.00	17.46	B	C
ATOM	10824	O	ILE	626	86.692	41.116	48.754	1.00	18.15	B	O
ATOM	10825	N	TRP	627	88.878	41.628	48.781	1.00	16.65	B	N
ATOM	10826	CA	TRP	627	88.663	42.938	48.177	1.00	15.95	B	C
ATOM	10827	CB	TRP	627	88.215	43.945	49.231	1.00	14.07	B	C
ATOM	10828	CG	TRP	627	89.318	44.713	49.875	1.00	12.00	B	C

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(Continued)

## FIG. 4 - 2 2 2

ATOM	10829	CD2	TRP	627	89.641	46.084	49.646	1.00	11.41	B	C
ATOM	10830	CE2	TRP	627	90.725	46.410	50.500	1.00	10.99	B	C
ATOM	10831	CE3	TRP	627	89.121	47.074	48.806	1.00	9.75	B	C
ATOM	10832	CD1	TRP	627	90.198	44.267	50.826	1.00	14.55	B	C
ATOM	10833	NE1	TRP	627	91.046	45.283	51.208	1.00	10.25	B	N
ATOM	10834	CZ2	TRP	627	91.289	47.681	50.536	1.00	9.06	B	C
ATOM	10835	CZ3	TRP	627	89.685	48.340	48.844	1.00	9.47	B	C
ATOM	10836	CH2	TRP	627	90.755	48.632	49.702	1.00	8.43	B	C
ATOM	10837	C	TRP	627	89.881	43.489	47.433	1.00	17.27	B	C
ATOM	10838	O	TRP	627	91.027	43.146	47.732	1.00	16.96	B	O
ATOM	10839	N	GLY	628	89.613	44.351	46.459	1.00	16.52	B	N
ATOM	10840	CA	GLY	628	90.672	44.947	45.675	1.00	16.52	B	C
ATOM	10841	C	GLY	628	90.186	46.198	44.975	1.00	17.44	B	C
ATOM	10842	O	GLY	628	88.977	46.441	44.887	1.00	17.88	B	O
ATOM	10843	N	TRP	629	91.132	46.989	44.479	1.00	15.93	B	N
ATOM	10844	CA	TRP	629	90.841	48.235	43.781	1.00	15.93	B	C
ATOM	10845	CB	TRP	629	91.480	49.395	44.552	1.00	13.57	B	C
ATOM	10846	CG	TRP	629	90.867	50.763	44.341	1.00	14.96	B	C
ATOM	10847	CD2	TRP	629	90.389	51.656	45.360	1.00	13.15	B	C
ATOM	10848	CE2	TRP	629	89.944	52.830	44.712	1.00	13.17	B	C
ATOM	10849	CE3	TRP	629	90.296	51.577	46.758	1.00	14.07	B	C
ATOM	10850	CD1	TRP	629	90.694	51.419	43.149	1.00	14.45	B	C
ATOM	10851	NE1	TRP	629	90.141	52.657	43.366	1.00	12.77	B	N
ATOM	10852	CZ2	TRP	629	89.411	53.921	45.414	1.00	13.59	B	C
ATOM	10853	CZ3	TRP	629	89.767	52.660	47.461	1.00	14.81	B	C
ATOM	10854	CH2	TRP	629	89.330	53.820	46.782	1.00	15.16	B	C
ATOM	10855	C	TRP	629	91.481	48.074	42.399	1.00	17.34	B	C
ATOM	10856	O	TRP	629	92.571	47.517	42.285	1.00	18.55	B	O
ATOM	10857	N	SER	630	90.802	48.538	41.354	1.00	17.70	B	N
ATOM	10858	CA	SER	630	91.309	48.430	39.982	1.00	17.70	B	C
ATOM	10859	CB	SER	630	92.649	49.144	39.846	1.00	18.19	B	C
ATOM	10860	OG	SER	630	92.574	50.437	40.404	1.00	24.67	B	O
ATOM	10861	C	SER	630	91.477	46.977	39.563	1.00	17.40	B	C
ATOM	10862	O	SER	630	90.501	46.235	39.469	1.00	18.69	B	O
ATOM	10863	N	TYR	631	92.712	46.565	39.304	1.00	16.34	B	N
ATOM	10864	CA	TYR	631	92.951	45.192	38.904	1.00	15.96	B	C
ATOM	10865	CB	TYR	631	94.430	44.973	38.579	1.00	15.36	B	C
ATOM	10866	CG	TYR	631	94.689	43.709	37.779	1.00	15.93	B	C
ATOM	10867	CD1	TYR	631	94.626	42.450	38.380	1.00	15.38	B	C
ATOM	10868	CE1	TYR	631	94.830	41.287	37.634	1.00	16.25	B	C
ATOM	10869	CD2	TYR	631	94.961	43.773	36.409	1.00	15.67	B	C
ATOM	10870	CE2	TYR	631	95.160	42.620	35.655	1.00	13.59	B	C
ATOM	10871	CZ	TYR	631	95.092	41.384	36.270	1.00	15.96	B	C
ATOM	10872	OH	TYR	631	95.264	40.243	35.525	1.00	14.59	B	O
ATOM	10873	C	TYR	631	92.499	44.286	40.049	1.00	15.68	B	C
ATOM	10874	O	TYR	631	91.949	43.213	39.824	1.00	16.42	B	O
ATOM	10875	N	GLY	632	92.723	44.729	41.281	1.00	15.56	B	N
ATOM	10876	CA	GLY	632	92.292	43.950	42.429	1.00	14.43	B	C
ATOM	10877	C	GLY	632	90.777	43.807	42.398	1.00	13.07	B	C

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(Continued)

## FIG. 4 - 2 2 3

ATOM	10878	O	GLY	632	90.239	42.771	42.777	1.00	12.09	B	O
ATOM	10879	N	GLY	633	90.087	44.855	41.946	1.00	12.57	B	N
ATOM	10880	CA	GLY	633	88.637	44.800	41.846	1.00	10.88	B	C
ATOM	10881	C	GLY	633	88.271	43.743	40.818	1.00	10.78	B	C
ATOM	10882	O	GLY	633	87.337	42.956	40.986	1.00	9.26	B	O
ATOM	10883	N	TYR	634	89.031	43.729	39.734	1.00	11.33	B	N
ATOM	10884	CA	TYR	634	88.822	42.755	38.682	1.00	11.09	B	C
ATOM	10885	CB	TYR	634	89.860	42.951	37.595	1.00	7.35	B	C
ATOM	10886	CG	TYR	634	89.815	41.899	36.526	1.00	8.04	B	C
ATOM	10887	CD1	TYR	634	90.949	41.162	36.204	1.00	7.58	B	C
ATOM	10888	CE1	TYR	634	90.924	40.218	35.189	1.00	7.56	B	C
ATOM	10889	CD2	TYR	634	88.649	41.660	35.805	1.00	8.82	B	C
ATOM	10890	CE2	TYR	634	88.615	40.715	34.788	1.00	7.88	B	C
ATOM	10891	CZ	TYR	634	89.756	39.996	34.488	1.00	6.90	B	C
ATOM	10892	OH	TYR	634	89.722	39.039	33.504	1.00	8.03	B	O
ATOM	10893	C	TYR	634	88.967	41.358	39.278	1.00	13.02	B	C
ATOM	10894	O	TYR	634	88.038	40.548	39.222	1.00	13.14	B	O
ATOM	10895	N	VAL	635	90.140	41.091	39.858	1.00	14.38	B	N
ATOM	10896	CA	VAL	635	90.426	39.796	40.467	1.00	13.39	B	C
ATOM	10897	CB	VAL	635	91.839	39.747	41.093	1.00	13.28	B	C
ATOM	10898	CG1	VAL	635	91.995	38.467	41.923	1.00	13.06	B	C
ATOM	10899	CG2	VAL	635	92.894	39.782	39.999	1.00	8.09	B	C
ATOM	10900	C	VAL	635	89.412	39.443	41.533	1.00	13.35	B	C
ATOM	10901	O	VAL	635	88.932	38.320	41.563	1.00	15.02	B	O
ATOM	10902	N	THR	636	89.091	40.394	42.405	1.00	13.48	B	N
ATOM	10903	CA	THR	636	88.108	40.160	43.457	1.00	13.74	B	C
ATOM	10904	CB	THR	636	87.788	41.451	44.260	1.00	15.19	B	C
ATOM	10905	OG1	THR	636	88.950	41.886	44.978	1.00	15.24	B	O
ATOM	10906	CG2	THR	636	86.655	41.188	45.259	1.00	13.51	B	C
ATOM	10907	C	THR	636	86.792	39.665	42.862	1.00	14.57	B	C
ATOM	10908	O	THR	636	86.160	38.750	43.395	1.00	15.29	B	O
ATOM	10909	N	SER	637	86.373	40.281	41.762	1.00	15.59	B	N
ATOM	10910	CA	SER	637	85.120	39.905	41.112	1.00	15.99	B	C
ATOM	10911	CB	SER	637	84.698	40.974	40.102	1.00	16.88	B	C
ATOM	10912	OG	SER	637	84.303	42.158	40.766	1.00	18.07	B	O
ATOM	10913	C	SER	637	85.195	38.558	40.420	1.00	16.54	B	C
ATOM	10914	O	SER	637	84.250	37.773	40.487	1.00	17.87	B	O
ATOM	10915	N	MET	638	86.309	38.300	39.740	1.00	15.64	B	N
ATOM	10916	CA	MET	638	86.493	37.030	39.052	1.00	15.55	B	C
ATOM	10917	CB	MET	638	87.807	37.033	38.272	1.00	15.97	B	C
ATOM	10918	CG	MET	638	87.822	37.959	37.067	1.00	17.38	B	C
ATOM	10919	SD	MET	638	86.715	37.422	35.736	1.00	19.14	B	S
ATOM	10920	CE	MET	638	87.806	36.324	34.798	1.00	15.28	B	C
ATOM	10921	C	MET	638	86.511	35.913	40.093	1.00	17.56	B	C
ATOM	10922	O	MET	638	86.018	34.807	39.843	1.00	17.45	B	O
ATOM	10923	N	VAL	639	87.086	36.199	41.260	1.00	16.50	B	N
ATOM	10924	CA	VAL	639	87.133	35.207	42.317	1.00	17.27	B	C
ATOM	10925	CB	VAL	639	88.047	35.640	43.480	1.00	16.78	B	C
ATOM	10926	CG1	VAL	639	87.648	34.884	44.757	1.00	16.23	B	C

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(Continued)

## FIG. 4 - 224

ATOM	10927	CG2	VAL	639	89.495	35.335	43.139	1.00	14.45	B	C
ATOM	10928	C	VAL	639	85.742	34.919	42.875	1.00	17.57	B	C
ATOM	10929	O	VAL	639	85.387	33.760	43.081	1.00	18.52	B	O
ATOM	10930	N	LEU	640	84.957	35.964	43.124	1.00	16.90	B	N
ATOM	10931	CA	LEU	640	83.618	35.766	43.661	1.00	17.42	B	C
ATOM	10932	CB	LEU	640	82.978	37.098	44.032	1.00	17.45	B	C
ATOM	10933	CG	LEU	640	83.512	37.699	45.327	1.00	17.52	B	C
ATOM	10934	CD1	LEU	640	82.743	38.962	45.654	1.00	14.30	B	C
ATOM	10935	CD2	LEU	640	83.378	36.677	46.447	1.00	15.97	B	C
ATOM	10936	C	LEU	640	82.713	35.020	42.699	1.00	17.81	B	C
ATOM	10937	O	LEU	640	81.821	34.284	43.119	1.00	20.73	B	O
ATOM	10938	N	GLY	641	82.952	35.198	41.409	1.00	18.14	B	N
ATOM	10939	CA	GLY	641	82.135	34.526	40.418	1.00	17.61	B	C
ATOM	10940	C	GLY	641	82.758	33.235	39.936	1.00	17.52	B	C
ATOM	10941	O	GLY	641	82.346	32.697	38.911	1.00	15.15	B	O
ATOM	10942	N	SER	642	83.735	32.727	40.683	1.00	17.53	B	N
ATOM	10943	CA	SER	642	84.419	31.497	40.297	1.00	19.98	B	C
ATOM	10944	CB	SER	642	85.841	31.479	40.864	1.00	20.78	B	C
ATOM	10945	OG	SER	642	85.849	31.088	42.226	1.00	21.56	B	O
ATOM	10946	C	SER	642	83.691	30.239	40.755	1.00	21.75	B	C
ATOM	10947	O	SER	642	83.974	29.147	40.265	1.00	22.65	B	O
ATOM	10948	N	GLY	643	82.768	30.395	41.701	1.00	22.05	B	N
ATOM	10949	CA	GLY	643	82.023	29.258	42.210	1.00	22.58	B	C
ATOM	10950	C	GLY	643	82.811	28.335	43.130	1.00	24.03	B	C
ATOM	10951	O	GLY	643	82.460	27.162	43.271	1.00	26.05	B	O
ATOM	10952	N	SER	644	83.859	28.849	43.772	1.00	22.41	B	N
ATOM	10953	CA	SER	644	84.684	28.024	44.656	1.00	21.56	B	C
ATOM	10954	CB	SER	644	86.065	28.657	44.833	1.00	21.02	B	C
ATOM	10955	OG	SER	644	85.992	29.798	45.666	1.00	22.35	B	O
ATOM	10956	C	SER	644	84.084	27.773	46.037	1.00	21.06	B	C
ATOM	10957	O	SER	644	84.451	26.807	46.707	1.00	23.51	B	O
ATOM	10958	N	GLY	645	83.175	28.643	46.469	1.00	19.50	B	N
ATOM	10959	CA	GLY	645	82.561	28.485	47.774	1.00	16.85	B	C
ATOM	10960	C	GLY	645	83.484	28.868	48.920	1.00	18.76	B	C
ATOM	10961	O	GLY	645	83.111	28.771	50.090	1.00	18.32	B	O
ATOM	10962	N	VAL	646	84.691	29.320	48.591	1.00	18.97	B	N
ATOM	10963	CA	VAL	646	85.669	29.695	49.612	1.00	18.18	B	C
ATOM	10964	CB	VAL	646	87.095	29.718	49.029	1.00	19.50	B	C
ATOM	10965	CG1	VAL	646	88.082	30.202	50.086	1.00	17.45	B	C
ATOM	10966	CG2	VAL	646	87.471	28.341	48.516	1.00	17.29	B	C
ATOM	10967	C	VAL	646	85.433	31.051	50.266	1.00	18.24	B	C
ATOM	10968	O	VAL	646	85.860	31.270	51.396	1.00	20.76	B	O
ATOM	10969	N	PHE	647	84.763	31.957	49.561	1.00	16.76	B	N
ATOM	10970	CA	PHE	647	84.525	33.297	50.082	1.00	16.60	B	C
ATOM	10971	CB	PHE	647	85.066	34.337	49.094	1.00	16.44	B	C
ATOM	10972	CG	PHE	647	86.528	34.204	48.820	1.00	15.63	B	C
ATOM	10973	CD1	PHE	647	87.455	34.941	49.553	1.00	14.72	B	C
ATOM	10974	CD2	PHE	647	86.985	33.320	47.844	1.00	14.49	B	C
ATOM	10975	CE1	PHE	647	88.826	34.800	49.317	1.00	16.66	B	C

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## FIG. 4 - 225

(Continued)

ATOM	10976	CE2	PHE	647	88.356	33.170	47.600	1.00	16.73	B	C
ATOM	10977	CZ	PHE	647	89.278	33.913	48.338	1.00	13.35	B	C
ATOM	10978	C	PHE	647	83.068	33.604	50.365	1.00	16.77	B	C
ATOM	10979	O	PHE	647	82.194	33.328	49.551	1.00	17.32	B	O
ATOM	10980	N	LYS	648	82.819	34.214	51.515	1.00	16.74	B	N
ATOM	10981	CA	LYS	648	81.466	34.565	51.905	1.00	19.64	B	C
ATOM	10982	CB	LYS	648	81.369	34.634	53.429	1.00	19.84	B	C
ATOM	10983	CG	LYS	648	80.069	35.233	53.911	1.00	21.93	B	C
ATOM	10984	CD	LYS	648	79.876	35.060	55.393	1.00	23.19	B	C
ATOM	10985	CE	LYS	648	78.548	35.645	55.814	1.00	24.97	B	C
ATOM	10986	NZ	LYS	648	78.180	35.150	57.165	1.00	31.55	B	N
ATOM	10987	C	LYS	648	81.019	35.900	51.308	1.00	21.05	B	C
ATOM	10988	O	LYS	648	79.851	36.070	50.930	1.00	20.25	B	O
ATOM	10989	N	CYS	649	81.954	36.842	51.237	1.00	20.69	B	N
ATOM	10990	CA	CYS	649	81.670	38.163	50.711	1.00	21.97	B	C
ATOM	10991	C	CYS	649	82.928	38.811	50.134	1.00	22.72	B	C
ATOM	10992	O	CYS	649	84.054	38.437	50.477	1.00	23.68	B	O
ATOM	10993	CB	CYS	649	81.124	39.045	51.822	1.00	23.52	B	C
ATOM	10994	SG	CYS	649	82.287	39.215	53.208	1.00	26.89	B	S
ATOM	10995	N	GLY	650	82.728	39.796	49.267	1.00	20.11	B	N
ATOM	10996	CA	GLY	650	83.850	40.476	48.668	1.00	18.42	B	C
ATOM	10997	C	GLY	650	83.484	41.895	48.308	1.00	18.08	B	C
ATOM	10998	O	GLY	650	82.308	42.198	48.135	1.00	18.19	B	O
ATOM	10999	N	ILE	651	84.490	42.764	48.209	1.00	17.42	B	N
ATOM	11000	CA	ILE	651	84.284	44.162	47.851	1.00	15.98	B	C
ATOM	11001	CB	ILE	651	84.632	45.117	49.014	1.00	15.40	B	C
ATOM	11002	CG2	ILE	651	84.386	46.559	48.589	1.00	15.87	B	C
ATOM	11003	CG1	ILE	651	83.789	44.786	50.242	1.00	15.95	B	C
ATOM	11004	CD1	ILE	651	84.017	45.721	51.411	1.00	14.84	B	C
ATOM	11005	C	ILE	651	85.190	44.512	46.679	1.00	16.40	B	C
ATOM	11006	O	ILE	651	86.404	44.330	46.754	1.00	16.63	B	O
ATOM	11007	N	ALA	652	84.594	45.025	45.608	1.00	16.04	B	N
ATOM	11008	CA	ALA	652	85.330	45.409	44.413	1.00	15.10	B	C
ATOM	11009	CB	ALA	652	84.809	44.629	43.214	1.00	16.38	B	C
ATOM	11010	C	ALA	652	85.190	46.908	44.153	1.00	15.88	B	C
ATOM	11011	O	ALA	652	84.089	47.399	43.895	1.00	14.37	B	O
ATOM	11012	N	VAL	653	86.308	47.630	44.214	1.00	15.73	B	N
ATOM	11013	CA	VAL	653	86.298	49.070	43.978	1.00	15.50	B	C
ATOM	11014	CB	VAL	653	87.110	49.831	45.055	1.00	17.97	B	C
ATOM	11015	CG1	VAL	653	87.050	51.327	44.787	1.00	18.06	B	C
ATOM	11016	CG2	VAL	653	86.566	49.525	46.446	1.00	18.80	B	C
ATOM	11017	C	VAL	653	86.905	49.398	42.624	1.00	15.11	B	C
ATOM	11018	O	VAL	653	88.071	49.087	42.373	1.00	14.41	B	O
ATOM	11019	N	ALA	654	86.106	50.031	41.766	1.00	14.05	B	N
ATOM	11020	CA	ALA	654	86.532	50.438	40.427	1.00	12.10	B	C
ATOM	11021	CB	ALA	654	87.424	51.655	40.518	1.00	12.15	B	C
ATOM	11022	C	ALA	654	87.258	49.318	39.700	1.00	12.48	B	C
ATOM	11023	O	ALA	654	88.364	49.500	39.192	1.00	13.17	B	O
ATOM	11024	N	PRO	655	86.633	48.141	39.626	1.00	11.84	B	N

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(Continued)

## FIG. 4 - 2 2 6

ATOM	11025	CD	PRO	655	85.273	47.797	40.088	1.00	11.50	B	C
ATOM	11026	CA	PRO	655	87.247	47.003	38.954	1.00	11.05	B	C
ATOM	11027	CB	PRO	655	86.399	45.841	39.436	1.00	11.09	B	C
ATOM	11028	CG	PRO	655	85.030	46.451	39.428	1.00	8.50	B	C
ATOM	11029	C	PRO	655	87.190	47.102	37.447	1.00	10.92	B	C
ATOM	11030	O	PRO	655	86.383	47.847	36.896	1.00	11.41	B	O
ATOM	11031	N	VAL	656	88.066	46.352	36.791	1.00	9.60	B	N
ATOM	11032	CA	VAL	656	88.052	46.250	35.345	1.00	9.08	B	C
ATOM	11033	CB	VAL	656	89.452	45.888	34.790	1.00	7.45	B	C
ATOM	11034	CG1	VAL	656	89.336	45.163	33.451	1.00	5.90	B	C
ATOM	11035	CG2	VAL	656	90.249	47.146	34.601	1.00	7.63	B	C
ATOM	11036	C	VAL	656	87.107	45.056	35.224	1.00	10.20	B	C
ATOM	11037	O	VAL	656	87.157	44.152	36.058	1.00	10.59	B	O
ATOM	11038	N	SER	657	86.231	45.038	34.230	1.00	11.76	B	N
ATOM	11039	CA	SER	657	85.313	43.908	34.115	1.00	14.03	B	C
ATOM	11040	CB	SER	657	83.867	44.375	34.271	1.00	13.85	B	C
ATOM	11041	OG	SER	657	83.495	45.242	33.218	1.00	15.07	B	O
ATOM	11042	C	SER	657	85.456	43.153	32.812	1.00	14.66	B	C
ATOM	11043	O	SER	657	85.191	41.952	32.743	1.00	17.18	B	O
ATOM	11044	N	ARG	658	85.887	43.860	31.781	1.00	14.15	B	N
ATOM	11045	CA	ARG	658	86.050	43.277	30.459	1.00	13.24	B	C
ATOM	11046	CB	ARG	658	84.768	43.532	29.670	1.00	14.22	B	C
ATOM	11047	CG	ARG	658	84.763	43.086	28.231	1.00	18.57	B	C
ATOM	11048	CD	ARG	658	83.436	43.470	27.588	1.00	19.40	B	C
ATOM	11049	NE	ARG	658	83.475	43.338	26.138	1.00	23.11	B	N
ATOM	11050	CZ	ARG	658	82.868	42.376	25.454	1.00	22.54	B	C
ATOM	11051	NH1	ARG	658	82.167	41.445	26.088	1.00	21.95	B	N
ATOM	11052	NH2	ARG	658	82.955	42.361	24.131	1.00	22.77	B	N
ATOM	11053	C	ARG	658	87.242	44.014	29.857	1.00	12.76	B	C
ATOM	11054	O	ARG	658	87.218	45.239	29.733	1.00	11.97	B	O
ATOM	11055	N	TRP	659	88.282	43.283	29.476	1.00	11.05	B	N
ATOM	11056	CA	TRP	659	89.468	43.942	28.955	1.00	12.23	B	C
ATOM	11057	CB	TRP	659	90.578	42.918	28.777	1.00	11.99	B	C
ATOM	11058	CG	TRP	659	91.026	42.392	30.112	1.00	13.26	B	C
ATOM	11059	CD2	TRP	659	91.729	43.120	31.122	1.00	12.61	B	C
ATOM	11060	CE2	TRP	659	91.848	42.271	32.242	1.00	13.22	B	C
ATOM	11061	CE3	TRP	659	92.268	44.412	31.193	1.00	14.19	B	C
ATOM	11062	CD1	TRP	659	90.759	41.163	30.644	1.00	13.17	B	C
ATOM	11063	NE1	TRP	659	91.247	41.083	31.920	1.00	13.29	B	N
ATOM	11064	CZ2	TRP	659	92.489	42.670	33.424	1.00	13.99	B	C
ATOM	11065	CZ3	TRP	659	92.909	44.810	32.373	1.00	13.35	B	C
ATOM	11066	CH2	TRP	659	93.011	43.940	33.468	1.00	11.92	B	C
ATOM	11067	C	TRP	659	89.338	44.840	27.730	1.00	13.23	B	C
ATOM	11068	O	TRP	659	90.118	45.766	27.569	1.00	15.39	B	O
ATOM	11069	N	GLU	660	88.361	44.595	26.871	1.00	14.59	B	N
ATOM	11070	CA	GLU	660	88.181	45.453	25.708	1.00	15.33	B	C
ATOM	11071	CB	GLU	660	87.147	44.854	24.743	1.00	18.10	B	C
ATOM	11072	CG	GLU	660	87.572	43.527	24.130	1.00	21.82	B	C
ATOM	11073	CD	GLU	660	86.452	42.829	23.386	1.00	25.49	B	C

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## FIG. 4 - 227

(Continued)

ATOM	11074	OE1	GLU	660	86.087	43.278	22.279	1.00	29.78	B	O
ATOM	11075	OE2	GLU	660	85.929	41.825	23.914	1.00	26.73	B	O
ATOM	11076	C	GLU	660	87.719	46.833	26.170	1.00	14.88	B	C
ATOM	11077	O	GLU	660	87.661	47.769	25.375	1.00	14.50	B	O
ATOM	11078	N	TYR	661	87.371	46.960	27.450	1.00	14.66	B	N
ATOM	11079	CA	TYR	661	86.941	48.258	27.977	1.00	15.13	B	C
ATOM	11080	CB	TYR	661	85.988	48.119	29.168	1.00	15.73	B	C
ATOM	11081	CG	TYR	661	84.599	47.597	28.872	1.00	19.12	B	C
ATOM	11082	CD1	TYR	661	83.823	47.053	29.898	1.00	18.37	B	C
ATOM	11083	CE1	TYR	661	82.553	46.548	29.653	1.00	19.84	B	C
ATOM	11084	CD2	TYR	661	84.061	47.629	27.581	1.00	19.07	B	C
ATOM	11085	CE2	TYR	661	82.782	47.123	27.323	1.00	20.28	B	C
ATOM	11086	CZ	TYR	661	82.035	46.581	28.367	1.00	20.80	B	C
ATOM	11087	OH	TYR	661	80.785	46.046	28.142	1.00	20.60	B	O
ATOM	11088	C	TYR	661	88.146	49.045	28.464	1.00	14.96	B	C
ATOM	11089	O	TYR	661	88.083	50.266	28.555	1.00	14.55	B	O
ATOM	11090	N	TYR	662	89.239	48.355	28.789	1.00	14.46	B	N
ATOM	11091	CA	TYR	662	90.411	49.060	29.289	1.00	15.14	B	C
ATOM	11092	CB	TYR	662	91.225	48.182	30.240	1.00	13.98	B	C
ATOM	11093	CG	TYR	662	92.049	49.021	31.187	1.00	14.52	B	C
ATOM	11094	CD1	TYR	662	93.379	48.699	31.468	1.00	14.22	B	C
ATOM	11095	CE1	TYR	662	94.168	49.531	32.255	1.00	11.31	B	C
ATOM	11096	CD2	TYR	662	91.522	50.194	31.734	1.00	13.44	B	C
ATOM	11097	CE2	TYR	662	92.297	51.030	32.520	1.00	13.70	B	C
ATOM	11098	CZ	TYR	662	93.620	50.699	32.776	1.00	13.69	B	C
ATOM	11099	OH	TYR	662	94.395	51.549	33.532	1.00	12.84	B	O
ATOM	11100	C	TYR	662	91.309	49.615	28.182	1.00	15.44	B	C
ATOM	11101	O	TYR	662	91.095	49.337	26.996	1.00	15.06	B	O
ATOM	11102	N	ASP	663	92.310	50.405	28.569	1.00	13.90	B	N
ATOM	11103	CA	ASP	663	93.192	51.026	27.588	1.00	13.58	B	C
ATOM	11104	CB	ASP	663	93.961	52.192	28.238	1.00	13.61	B	C
ATOM	11105	CG	ASP	663	95.093	51.741	29.152	1.00	14.10	B	C
ATOM	11106	OD1	ASP	663	95.223	52.327	30.243	1.00	12.30	B	O
ATOM	11107	OD2	ASP	663	95.869	50.836	28.780	1.00	13.70	B	O
ATOM	11108	C	ASP	663	94.139	50.076	26.850	1.00	13.21	B	C
ATOM	11109	O	ASP	663	94.565	49.045	27.378	1.00	13.05	B	O
ATOM	11110	N	SER	664	94.453	50.444	25.612	1.00	13.86	B	N
ATOM	11111	CA	SER	664	95.321	49.658	24.738	1.00	13.65	B	C
ATOM	11112	CB	SER	664	95.464	50.364	23.394	1.00	14.44	B	C
ATOM	11113	OG	SER	664	96.055	51.642	23.550	1.00	16.79	B	O
ATOM	11114	C	SER	664	96.714	49.340	25.278	1.00	13.42	B	C
ATOM	11115	O	SER	664	97.066	48.176	25.438	1.00	12.83	B	O
ATOM	11116	N	VAL	665	97.503	50.371	25.559	1.00	12.98	B	N
ATOM	11117	CA	VAL	665	98.865	50.158	26.041	1.00	15.86	B	C
ATOM	11118	CB	VAL	665	99.547	51.496	26.427	1.00	14.66	B	C
ATOM	11119	CG1	VAL	665	101.023	51.263	26.663	1.00	14.68	B	C
ATOM	11120	CG2	VAL	665	99.354	52.519	25.327	1.00	15.28	B	C
ATOM	11121	C	VAL	665	99.020	49.169	27.206	1.00	15.25	B	C
ATOM	11122	O	VAL	665	99.972	48.400	27.242	1.00	15.22	B	O

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(Continued)

## FIG. 4 - 228

ATOM	11123	N	TYR	666	98.091	49.184	28.154	1.00	17.07	B	N
ATOM	11124	CA	TYR	666	98.175	48.276	29.299	1.00	15.32	B	C
ATOM	11125	CB	TYR	666	97.504	48.896	30.531	1.00	13.28	B	C
ATOM	11126	CG	TYR	666	97.483	47.997	31.751	1.00	12.79	B	C
ATOM	11127	CD1	TYR	666	96.595	46.920	31.845	1.00	12.27	B	C
ATOM	11128	CE1	TYR	666	96.583	46.089	32.964	1.00	12.60	B	C
ATOM	11129	CD2	TYR	666	98.360	48.215	32.809	1.00	12.83	B	C
ATOM	11130	CE2	TYR	666	98.361	47.390	33.928	1.00	11.79	B	C
ATOM	11131	CZ	TYR	666	97.472	46.332	34.005	1.00	13.90	B	C
ATOM	11132	OH	TYR	666	97.471	45.531	35.131	1.00	12.51	B	O
ATOM	11133	C	TYR	666	97.550	46.922	29.023	1.00	15.26	B	C
ATOM	11134	O	TYR	666	98.103	45.895	29.399	1.00	18.30	B	O
ATOM	11135	N	THR	667	96.401	46.912	28.365	1.00	14.70	B	N
ATOM	11136	CA	THR	667	95.712	45.656	28.097	1.00	13.70	B	C
ATOM	11137	CB	THR	667	94.264	45.925	27.656	1.00	12.07	B	C
ATOM	11138	OG1	THR	667	93.617	46.756	28.635	1.00	11.17	B	O
ATOM	11139	CG2	THR	667	93.498	44.624	27.533	1.00	10.21	B	C
ATOM	11140	C	THR	667	96.423	44.792	27.067	1.00	15.29	B	C
ATOM	11141	O	THR	667	96.713	43.626	27.323	1.00	16.16	B	O
ATOM	11142	N	GLU	668	96.707	45.372	25.906	1.00	16.99	B	N
ATOM	11143	CA	GLU	668	97.389	44.672	24.823	1.00	16.90	B	C
ATOM	11144	CB	GLU	668	97.537	45.612	23.625	1.00	17.50	B	C
ATOM	11145	CG	GLU	668	96.231	45.808	22.867	1.00	21.31	B	C
ATOM	11146	CD	GLU	668	96.275	46.928	21.850	1.00	22.06	B	C
ATOM	11147	OE1	GLU	668	97.284	47.054	21.123	1.00	25.39	B	O
ATOM	11148	OE2	GLU	668	95.284	47.679	21.767	1.00	22.03	B	O
ATOM	11149	C	GLU	668	98.751	44.127	25.247	1.00	17.77	B	C
ATOM	11150	O	GLU	668	99.186	43.079	24.766	1.00	19.28	B	O
ATOM	11151	N	ARG	669	99.418	44.827	26.158	1.00	17.62	B	N
ATOM	11152	CA	ARG	669	100.721	44.392	26.640	1.00	17.00	B	C
ATOM	11153	CB	ARG	669	101.199	45.291	27.785	1.00	17.11	B	C
ATOM	11154	CG	ARG	669	102.498	44.828	28.451	1.00	15.99	B	C
ATOM	11155	CD	ARG	669	102.878	45.766	29.583	1.00	15.35	B	C
ATOM	11156	NE	ARG	669	102.914	47.149	29.122	1.00	16.25	B	N
ATOM	11157	CZ	ARG	669	102.549	48.196	29.856	1.00	16.96	B	C
ATOM	11158	NH1	ARG	669	102.115	48.023	31.101	1.00	16.86	B	N
ATOM	11159	NH2	ARG	669	102.602	49.417	29.340	1.00	14.86	B	N
ATOM	11160	C	ARG	669	100.633	42.960	27.140	1.00	17.70	B	C
ATOM	11161	O	ARG	669	101.523	42.141	26.899	1.00	17.72	B	O
ATOM	11162	N	TYR	670	99.539	42.655	27.825	1.00	17.60	B	N
ATOM	11163	CA	TYR	670	99.357	41.333	28.385	1.00	16.56	B	C
ATOM	11164	CB	TYR	670	98.823	41.465	29.810	1.00	15.82	B	C
ATOM	11165	CG	TYR	670	99.571	42.491	30.631	1.00	15.47	B	C
ATOM	11166	CD1	TYR	670	98.978	43.706	30.973	1.00	14.06	B	C
ATOM	11167	CE1	TYR	670	99.680	44.676	31.676	1.00	14.36	B	C
ATOM	11168	CD2	TYR	670	100.894	42.268	31.024	1.00	15.93	B	C
ATOM	11169	CE2	TYR	670	101.608	43.232	31.732	1.00	15.78	B	C
ATOM	11170	CZ	TYR	670	100.998	44.433	32.051	1.00	15.30	B	C
ATOM	11171	OH	TYR	670	101.713	45.403	32.714	1.00	15.22	B	O

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(Continued)

## FIG. 4 - 229

ATOM	11172	C	TYR	670	98.435	40.441	27.578	1.00	17.87	B	C
ATOM	11173	O	TYR	670	98.637	39.231	27.508	1.00	18.02	B	O
ATOM	11174	N	MET	671	97.435	41.040	26.948	1.00	18.57	B	N
ATOM	11175	CA	MET	671	96.452	40.271	26.199	1.00	19.04	B	C
ATOM	11176	CB	MET	671	95.063	40.844	26.482	1.00	21.47	B	C
ATOM	11177	CG	MET	671	94.604	40.692	27.919	1.00	21.74	B	C
ATOM	11178	SD	MET	671	94.228	38.972	28.277	1.00	28.61	B	S
ATOM	11179	CE	MET	671	92.570	38.871	27.582	1.00	23.84	B	C
ATOM	11180	C	MET	671	96.640	40.164	24.692	1.00	19.95	B	C
ATOM	11181	O	MET	671	96.121	39.240	24.075	1.00	20.85	B	O
ATOM	11182	N	GLY	672	97.380	41.092	24.094	1.00	20.28	B	N
ATOM	11183	CA	GLY	672	97.540	41.063	22.654	1.00	19.08	B	C
ATOM	11184	C	GLY	672	96.354	41.807	22.068	1.00	21.12	B	C
ATOM	11185	O	GLY	672	95.746	42.629	22.755	1.00	21.18	B	O
ATOM	11186	N	LEU	673	96.009	41.534	20.814	1.00	21.68	B	N
ATOM	11187	CA	LEU	673	94.884	42.225	20.186	1.00	21.44	B	C
ATOM	11188	CB	LEU	673	95.204	42.569	18.732	1.00	22.03	B	C
ATOM	11189	CG	LEU	673	96.287	43.627	18.507	1.00	24.89	B	C
ATOM	11190	CD1	LEU	673	96.518	43.837	17.023	1.00	23.45	B	C
ATOM	11191	CD2	LEU	673	95.846	44.932	19.150	1.00	27.67	B	C
ATOM	11192	C	LEU	673	93.616	41.399	20.243	1.00	21.68	B	C
ATOM	11193	O	LEU	673	93.647	40.173	20.076	1.00	21.49	B	O
ATOM	11194	N	PRO	674	92.475	42.061	20.487	1.00	21.61	B	N
ATOM	11195	CD	PRO	674	92.342	43.487	20.830	1.00	20.79	B	C
ATOM	11196	CA	PRO	674	91.180	41.388	20.571	1.00	20.99	B	C
ATOM	11197	CB	PRO	674	90.365	42.347	21.420	1.00	19.09	B	C
ATOM	11198	CG	PRO	674	90.845	43.664	20.941	1.00	18.24	B	C
ATOM	11199	C	PRO	674	90.589	41.155	19.183	1.00	21.53	B	C
ATOM	11200	O	PRO	674	89.470	41.561	18.884	1.00	20.30	B	O
ATOM	11201	N	THR	675	91.378	40.505	18.335	1.00	23.61	B	N
ATOM	11202	CA	THR	675	90.973	40.176	16.975	1.00	23.43	B	C
ATOM	11203	CB	THR	675	92.045	40.560	15.957	1.00	22.99	B	C
ATOM	11204	OG1	THR	675	93.221	39.783	16.200	1.00	24.15	B	O
ATOM	11205	CG2	THR	675	92.386	42.039	16.062	1.00	21.26	B	C
ATOM	11206	C	THR	675	90.825	38.668	16.931	1.00	25.46	B	C
ATOM	11207	O	THR	675	91.424	37.952	17.736	1.00	25.82	B	O
ATOM	11208	N	PRO	676	90.023	38.160	15.991	1.00	26.60	B	N
ATOM	11209	CD	PRO	676	89.130	38.885	15.074	1.00	25.76	B	C
ATOM	11210	CA	PRO	676	89.823	36.714	15.877	1.00	26.64	B	C
ATOM	11211	CB	PRO	676	88.860	36.599	14.702	1.00	25.84	B	C
ATOM	11212	CG	PRO	676	88.066	37.859	14.801	1.00	24.99	B	C
ATOM	11213	C	PRO	676	91.135	35.967	15.630	1.00	28.63	B	C
ATOM	11214	O	PRO	676	91.347	34.875	16.160	1.00	28.85	B	O
ATOM	11215	N	GLU	677	92.021	36.557	14.834	1.00	30.55	B	N
ATOM	11216	CA	GLU	677	93.286	35.905	14.534	1.00	31.94	B	C
ATOM	11217	CB	GLU	677	93.772	36.290	13.135	1.00	35.44	B	C
ATOM	11218	CG	GLU	677	94.177	35.077	12.294	1.00	41.76	B	C
ATOM	11219	CD	GLU	677	92.984	34.204	11.897	1.00	46.15	B	C
ATOM	11220	OE1	GLU	677	92.234	34.610	10.980	1.00	49.52	B	O

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(Continued)

## FIG. 4 - 230

ATOM	11221	OE2	GLU	677	92.789	33.121	12.503	1.00	46.47	B	O
ATOM	11222	C	GLU	677	94.382	36.174	15.563	1.00	31.51	B	C
ATOM	11223	O	GLU	677	95.565	35.938	15.305	1.00	31.18	B	O
ATOM	11224	N	ASP	678	94.003	36.680	16.730	1.00	29.04	B	N
ATOM	11225	CA	ASP	678	95.005	36.896	17.756	1.00	26.71	B	C
ATOM	11226	CB	ASP	678	95.359	38.374	17.917	1.00	25.30	B	C
ATOM	11227	CG	ASP	678	96.500	38.586	18.902	1.00	26.53	B	C
ATOM	11228	OD1	ASP	678	97.004	39.721	19.008	1.00	29.18	B	O
ATOM	11229	OD2	ASP	678	96.900	37.612	19.579	1.00	24.47	B	O
ATOM	11230	C	ASP	678	94.586	36.325	19.098	1.00	25.24	B	C
ATOM	11231	O	ASP	678	94.946	35.200	19.426	1.00	26.23	B	O
ATOM	11232	N	ASN	679	93.814	37.082	19.871	1.00	24.14	B	N
ATOM	11233	CA	ASN	679	93.418	36.608	21.186	1.00	22.47	B	C
ATOM	11234	CB	ASN	679	94.456	37.089	22.217	1.00	23.05	B	C
ATOM	11235	CG	ASN	679	94.390	36.323	23.524	1.00	22.50	B	C
ATOM	11236	OD1	ASN	679	94.644	36.880	24.592	1.00	21.44	B	O
ATOM	11237	ND2	ASN	679	94.059	35.037	23.448	1.00	22.30	B	N
ATOM	11238	C	ASN	679	92.019	37.061	21.596	1.00	21.85	B	C
ATOM	11239	O	ASN	679	91.727	37.174	22.785	1.00	21.56	B	O
ATOM	11240	N	LEU	680	91.153	37.316	20.619	1.00	22.96	B	N
ATOM	11241	CA	LEU	680	89.783	37.750	20.913	1.00	22.05	B	C
ATOM	11242	CB	LEU	680	88.999	37.967	19.617	1.00	20.94	B	C
ATOM	11243	CG	LEU	680	87.524	38.379	19.734	1.00	20.98	B	C
ATOM	11244	CD1	LEU	680	87.385	39.671	20.539	1.00	21.18	B	C
ATOM	11245	CD2	LEU	680	86.946	38.567	18.348	1.00	17.15	B	C
ATOM	11246	C	LEU	680	89.031	36.762	21.805	1.00	22.36	B	C
ATOM	11247	O	LEU	680	88.316	37.171	22.718	1.00	23.81	B	O
ATOM	11248	N	ASP	681	89.193	35.466	21.555	1.00	22.95	B	N
ATOM	11249	CA	ASP	681	88.502	34.469	22.371	1.00	24.27	B	C
ATOM	11250	CB	ASP	681	88.910	33.048	21.980	1.00	24.73	B	C
ATOM	11251	CG	ASP	681	88.270	32.587	20.695	1.00	25.98	B	C
ATOM	11252	OD1	ASP	681	87.453	33.334	20.116	1.00	28.21	B	O
ATOM	11253	OD2	ASP	681	88.587	31.462	20.259	1.00	28.60	B	O
ATOM	11254	C	ASP	681	88.754	34.655	23.862	1.00	23.99	B	C
ATOM	11255	O	ASP	681	87.816	34.640	24.660	1.00	24.77	B	O
ATOM	11256	N	HIS	682	90.014	34.819	24.252	1.00	22.66	B	N
ATOM	11257	CA	HIS	682	90.289	34.998	25.667	1.00	22.62	B	C
ATOM	11258	CB	HIS	682	91.775	34.867	25.981	1.00	23.03	B	C
ATOM	11259	CG	HIS	682	92.063	34.898	27.448	1.00	25.79	B	C
ATOM	11260	CD2	HIS	682	92.844	35.718	28.190	1.00	26.73	B	C
ATOM	11261	ND1	HIS	682	91.458	34.035	28.338	1.00	25.30	B	N
ATOM	11262	CE1	HIS	682	91.852	34.326	29.565	1.00	26.50	B	C
ATOM	11263	NE2	HIS	682	92.693	35.344	29.504	1.00	26.09	B	N
ATOM	11264	C	HIS	682	89.775	36.344	26.175	1.00	21.71	B	C
ATOM	11265	O	HIS	682	89.412	36.465	27.345	1.00	20.98	B	O
ATOM	11266	N	TYR	683	89.753	37.355	25.307	1.00	19.91	B	N
ATOM	11267	CA	TYR	683	89.232	38.657	25.707	1.00	19.50	B	C
ATOM	11268	CB	TYR	683	89.226	39.646	24.542	1.00	16.55	B	C
ATOM	11269	CG	TYR	683	90.419	40.574	24.472	1.00	16.85	B	C

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## FIG. 4 - 231

(Continued)

ATOM	11270	CD1	TYR	683	91.616	40.172	23.877	1.00	16.29	B	C
ATOM	11271	CE1	TYR	683	92.700	41.040	23.786	1.00	16.38	B	C
ATOM	11272	CD2	TYR	683	90.345	41.871	24.980	1.00	16.79	B	C
ATOM	11273	CE2	TYR	683	91.430	42.748	24.893	1.00	14.60	B	C
ATOM	11274	CZ	TYR	683	92.598	42.326	24.295	1.00	15.79	B	C
ATOM	11275	OH	TYR	683	93.663	43.193	24.192	1.00	16.43	B	O
ATOM	11276	C	TYR	683	87.793	38.437	26.150	1.00	21.02	B	C
ATOM	11277	O	TYR	683	87.355	38.955	27.174	1.00	20.95	B	O
ATOM	11278	N	ARG	684	87.071	37.644	25.367	1.00	22.94	B	N
ATOM	11279	CA	ARG	684	85.667	37.349	25.634	1.00	24.36	B	C
ATOM	11280	CB	ARG	684	84.992	36.871	24.344	1.00	24.11	B	C
ATOM	11281	CG	ARG	684	84.996	37.908	23.234	1.00	25.07	B	C
ATOM	11282	CD	ARG	684	84.197	39.132	23.639	1.00	25.30	B	C
ATOM	11283	NE	ARG	684	84.453	40.275	22.767	1.00	27.33	B	N
ATOM	11284	CZ	ARG	684	84.126	40.344	21.480	1.00	27.26	B	C
ATOM	11285	NH1	ARG	684	83.518	39.327	20.880	1.00	27.78	B	N
ATOM	11286	NH2	ARG	684	84.409	41.443	20.794	1.00	26.25	B	N
ATOM	11287	C	ARG	684	85.401	36.340	26.745	1.00	24.46	B	C
ATOM	11288	O	ARG	684	84.275	36.239	27.231	1.00	26.21	B	O
ATOM	11289	N	ASN	685	86.421	35.591	27.148	1.00	24.53	B	N
ATOM	11290	CA	ASN	685	86.243	34.593	28.201	1.00	23.44	B	C
ATOM	11291	CB	ASN	685	86.959	33.294	27.823	1.00	26.13	B	C
ATOM	11292	CG	ASN	685	86.132	32.430	26.904	1.00	33.00	B	C
ATOM	11293	OD1	ASN	685	85.076	31.924	27.296	1.00	35.72	B	O
ATOM	11294	ND2	ASN	685	86.594	32.260	25.667	1.00	36.03	B	N
ATOM	11295	C	ASN	685	86.716	35.043	29.575	1.00	20.60	B	C
ATOM	11296	O	ASN	685	86.472	34.361	30.566	1.00	20.98	B	O
ATOM	11297	N	SER	686	87.382	36.186	29.644	1.00	16.28	B	N
ATOM	11298	CA	SER	686	87.887	36.666	30.918	1.00	16.33	B	C
ATOM	11299	CB	SER	686	89.360	37.063	30.773	1.00	17.18	B	C
ATOM	11300	OG	SER	686	89.530	38.050	29.768	1.00	17.94	B	O
ATOM	11301	C	SER	686	87.089	37.837	31.486	1.00	15.71	B	C
ATOM	11302	O	SER	686	87.625	38.667	32.221	1.00	13.91	B	O
ATOM	11303	N	THR	687	85.807	37.905	31.155	1.00	14.37	B	N
ATOM	11304	CA	THR	687	84.989	38.992	31.655	1.00	15.19	B	C
ATOM	11305	CB	THR	687	83.899	39.401	30.639	1.00	16.80	B	C
ATOM	11306	OG1	THR	687	82.915	38.362	30.537	1.00	18.14	B	O
ATOM	11307	CG2	THR	687	84.519	39.657	29.265	1.00	16.92	B	C
ATOM	11308	C	THR	687	84.309	38.605	32.957	1.00	14.86	B	C
ATOM	11309	O	THR	687	84.153	37.425	33.264	1.00	13.79	B	O
ATOM	11310	N	VAL	688	83.910	39.616	33.717	1.00	14.71	B	N
ATOM	11311	CA	VAL	688	83.224	39.411	34.977	1.00	14.27	B	C
ATOM	11312	CB	VAL	688	83.239	40.691	35.824	1.00	15.67	B	C
ATOM	11313	CG1	VAL	688	82.476	40.464	37.130	1.00	15.43	B	C
ATOM	11314	CG2	VAL	688	84.687	41.115	36.100	1.00	18.49	B	C
ATOM	11315	C	VAL	688	81.777	39.048	34.687	1.00	14.74	B	C
ATOM	11316	O	VAL	688	81.196	38.188	35.350	1.00	15.40	B	O
ATOM	11317	N	MET	689	81.209	39.710	33.682	1.00	13.94	B	N
ATOM	11318	CA	MET	689	79.826	39.496	33.283	1.00	14.18	B	C

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(Continued)

## FIG. 4 - 232

ATOM	11319	CB	MET	689	79.519	40.287	32.010	1.00	14.10	B	C
ATOM	11320	CG	MET	689	79.359	41.793	32.217	1.00	18.18	B	C
ATOM	11321	SD	MET	689	80.817	42.684	32.849	1.00	21.67	B	S
ATOM	11322	CE	MET	689	81.693	43.067	31.308	1.00	19.11	B	C
ATOM	11323	C	MET	689	79.429	38.040	33.080	1.00	13.66	B	C
ATOM	11324	O	MET	689	78.398	37.597	33.586	1.00	14.01	B	O
ATOM	11325	N	SER	690	80.246	37.290	32.356	1.00	14.32	B	N
ATOM	11326	CA	SER	690	79.939	35.887	32.087	1.00	16.68	B	C
ATOM	11327	CB	SER	690	81.018	35.259	31.199	1.00	18.28	B	C
ATOM	11328	OG	SER	690	82.225	35.062	31.923	1.00	23.11	B	O
ATOM	11329	C	SER	690	79.771	35.019	33.328	1.00	15.55	B	C
ATOM	11330	O	SER	690	79.212	33.927	33.234	1.00	16.21	B	O
ATOM	11331	N	ARG	691	80.238	35.502	34.478	1.00	14.35	B	N
ATOM	11332	CA	ARG	691	80.155	34.741	35.727	1.00	15.38	B	C
ATOM	11333	CB	ARG	691	81.491	34.821	36.478	1.00	16.76	B	C
ATOM	11334	CG	ARG	691	82.697	34.414	35.652	1.00	19.96	B	C
ATOM	11335	CD	ARG	691	83.972	34.339	36.483	1.00	21.36	B	C
ATOM	11336	NE	ARG	691	85.061	33.725	35.726	1.00	23.56	B	N
ATOM	11337	CZ	ARG	691	86.196	33.274	36.256	1.00	26.24	B	C
ATOM	11338	NH1	ARG	691	86.418	33.358	37.567	1.00	23.55	B	N
ATOM	11339	NH2	ARG	691	87.114	32.728	35.468	1.00	26.33	B	N
ATOM	11340	C	ARG	691	79.049	35.187	36.679	1.00	15.48	B	C
ATOM	11341	O	ARG	691	78.986	34.713	37.817	1.00	14.38	B	O
ATOM	11342	N	ALA	692	78.178	36.081	36.220	1.00	14.78	B	N
ATOM	11343	CA	ALA	692	77.111	36.618	37.064	1.00	16.42	B	C
ATOM	11344	CB	ALA	692	76.105	37.383	36.198	1.00	16.75	B	C
ATOM	11345	C	ALA	692	76.375	35.624	37.977	1.00	17.17	B	C
ATOM	11346	O	ALA	692	76.331	35.814	39.191	1.00	16.75	B	O
ATOM	11347	N	GLU	693	75.803	34.571	37.404	1.00	19.44	B	N
ATOM	11348	CA	GLU	693	75.062	33.589	38.191	1.00	22.16	B	C
ATOM	11349	CB	GLU	693	74.570	32.443	37.299	1.00	26.71	B	C
ATOM	11350	CG	GLU	693	73.251	32.745	36.598	1.00	33.79	B	C
ATOM	11351	CD	GLU	693	73.017	31.873	35.379	1.00	38.47	B	C
ATOM	11352	OE1	GLU	693	72.984	30.632	35.531	1.00	40.41	B	O
ATOM	11353	OE2	GLU	693	72.870	32.433	34.266	1.00	41.15	B	O
ATOM	11354	C	GLU	693	75.827	33.022	39.369	1.00	22.08	B	C
ATOM	11355	O	GLU	693	75.244	32.761	40.418	1.00	24.44	B	O
ATOM	11356	N	ASN	694	77.127	32.824	39.215	1.00	21.66	B	N
ATOM	11357	CA	ASN	694	77.907	32.282	40.320	1.00	22.61	B	C
ATOM	11358	CB	ASN	694	79.324	31.924	39.861	1.00	20.93	B	C
ATOM	11359	CG	ASN	694	79.359	30.654	39.048	1.00	19.32	B	C
ATOM	11360	OD1	ASN	694	80.284	30.420	38.278	1.00	19.68	B	O
ATOM	11361	ND2	ASN	694	78.348	29.818	39.224	1.00	18.34	B	N
ATOM	11362	C	ASN	694	77.975	33.234	41.500	1.00	22.99	B	C
ATOM	11363	O	ASN	694	78.650	32.946	42.479	1.00	25.59	B	O
ATOM	11364	N	PHE	695	77.283	34.366	41.419	1.00	22.83	B	N
ATOM	11365	CA	PHE	695	77.299	35.316	42.531	1.00	23.74	B	C
ATOM	11366	CB	PHE	695	77.205	36.772	42.041	1.00	20.88	B	C
ATOM	11367	CG	PHE	695	78.533	37.397	41.695	1.00	19.06	B	C

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(Continued)

## FIG. 4 - 233

ATOM	11368	CD1 PHE	695	79.211	37.042	40.533	1.00	19.50	B	C
ATOM	11369	CD2 PHE	695	79.096	38.365	42.523	1.00	19.69	B	C
ATOM	11370	CE1 PHE	695	80.431	37.647	40.200	1.00	18.29	B	C
ATOM	11371	CE2 PHE	695	80.316	38.977	42.199	1.00	18.53	B	C
ATOM	11372	CZ PHE	695	80.982	38.615	41.033	1.00	17.35	B	C
ATOM	11373	C PHE	695	76.146	35.052	43.483	1.00	24.37	B	C
ATOM	11374	O PHE	695	76.090	35.636	44.566	1.00	25.67	B	O
ATOM	11375	N LYS	696	75.230	34.173	43.089	1.00	24.40	B	N
ATOM	11376	CA LYS	696	74.074	33.880	43.926	1.00	25.82	B	C
ATOM	11377	CB LYS	696	73.173	32.813	43.280	1.00	27.75	B	C
ATOM	11378	CG LYS	696	72.076	32.281	44.228	1.00	30.02	B	C
ATOM	11379	CD LYS	696	70.680	32.287	43.615	1.00	31.63	B	C
ATOM	11380	CE LYS	696	70.137	33.705	43.421	1.00	35.45	B	C
ATOM	11381	NZ LYS	696	69.903	34.438	44.705	1.00	35.47	B	N
ATOM	11382	C LYS	696	74.402	33.459	45.348	1.00	24.85	B	C
ATOM	11383	O LYS	696	73.583	33.641	46.242	1.00	24.94	B	O
ATOM	11384	N GLN	697	75.587	32.907	45.577	1.00	25.99	B	N
ATOM	11385	CA GLN	697	75.920	32.481	46.931	1.00	27.33	B	C
ATOM	11386	CB GLN	697	76.355	31.010	46.941	1.00	29.90	B	C
ATOM	11387	CG GLN	697	75.290	30.025	46.444	1.00	30.66	B	C
ATOM	11388	CD GLN	697	75.565	28.593	46.889	1.00	30.92	B	C
ATOM	11389	OE1 GLN	697	75.381	28.245	48.065	1.00	31.54	B	O
ATOM	11390	NE2 GLN	697	76.019	27.761	45.958	1.00	26.21	B	N
ATOM	11391	C GLN	697	76.964	33.322	47.662	1.00	26.04	B	C
ATOM	11392	O GLN	697	77.620	32.833	48.580	1.00	28.31	B	O
ATOM	11393	N VAL	698	77.125	34.580	47.270	1.00	23.16	B	N
ATOM	11394	CA VAL	698	78.085	35.445	47.947	1.00	21.23	B	C
ATOM	11395	CB VAL	698	79.411	35.596	47.156	1.00	20.63	B	C
ATOM	11396	CG1 VAL	698	80.033	34.238	46.901	1.00	17.19	B	C
ATOM	11397	CG2 VAL	698	79.161	36.335	45.853	1.00	18.36	B	C
ATOM	11398	C VAL	698	77.496	36.829	48.118	1.00	21.50	B	C
ATOM	11399	O VAL	698	76.571	37.207	47.404	1.00	23.06	B	O
ATOM	11400	N GLU	699	78.018	37.579	49.078	1.00	21.31	B	N
ATOM	11401	CA GLU	699	77.563	38.945	49.290	1.00	21.42	B	C
ATOM	11402	CB GLU	699	77.465	39.246	50.785	1.00	22.73	B	C
ATOM	11403	CG GLU	699	76.396	38.403	51.461	1.00	26.07	B	C
ATOM	11404	CD GLU	699	76.547	38.346	52.961	1.00	29.09	B	C
ATOM	11405	OE1 GLU	699	76.343	39.387	53.624	1.00	31.29	B	O
ATOM	11406	OE2 GLU	699	76.876	37.254	53.476	1.00	31.07	B	O
ATOM	11407	C GLU	699	78.610	39.810	48.593	1.00	21.23	B	C
ATOM	11408	O GLU	699	79.802	39.751	48.905	1.00	21.45	B	O
ATOM	11409	N TYR	700	78.148	40.594	47.630	1.00	19.47	B	N
ATOM	11410	CA TYR	700	79.012	41.428	46.818	1.00	18.26	B	C
ATOM	11411	CB TYR	700	78.830	41.001	45.368	1.00	18.24	B	C
ATOM	11412	CG TYR	700	79.678	41.685	44.330	1.00	18.56	B	C
ATOM	11413	CD1 TYR	700	81.071	41.698	44.422	1.00	17.75	B	C
ATOM	11414	CE1 TYR	700	81.856	42.206	43.378	1.00	17.99	B	C
ATOM	11415	CD2 TYR	700	79.088	42.209	43.181	1.00	19.07	B	C
ATOM	11416	CE2 TYR	700	79.852	42.715	42.143	1.00	19.54	B	C

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(Continued)

## FIG. 4 - 234

ATOM	11417	CZ	TYR	700	81.231	42.707	42.241	1.00	19.61	B	C
ATOM	11418	OH	TYR	700	81.964	43.170	41.176	1.00	20.17	B	O
ATOM	11419	C	TYR	700	78.697	42.902	46.972	1.00	18.20	B	C
ATOM	11420	O	TYR	700	77.534	43.288	47.006	1.00	19.67	B	O
ATOM	11421	N	LEU	701	79.748	43.714	47.078	1.00	16.71	B	N
ATOM	11422	CA	LEU	701	79.628	45.157	47.198	1.00	15.24	B	C
ATOM	11423	CB	LEU	701	80.102	45.624	48.573	1.00	14.82	B	C
ATOM	11424	CG	LEU	701	80.195	47.141	48.768	1.00	15.42	B	C
ATOM	11425	CD1	LEU	701	78.926	47.810	48.280	1.00	16.37	B	C
ATOM	11426	CD2	LEU	701	80.449	47.456	50.233	1.00	13.32	B	C
ATOM	11427	C	LEU	701	80.491	45.770	46.095	1.00	16.15	B	C
ATOM	11428	O	LEU	701	81.714	45.617	46.082	1.00	16.12	B	O
ATOM	11429	N	LEU	702	79.829	46.450	45.167	1.00	14.91	B	N
ATOM	11430	CA	LEU	702	80.467	47.073	44.019	1.00	13.94	B	C
ATOM	11431	CB	LEU	702	79.730	46.627	42.753	1.00	15.12	B	C
ATOM	11432	CG	LEU	702	80.119	47.175	41.383	1.00	15.68	B	C
ATOM	11433	CD1	LEU	702	81.555	46.814	41.050	1.00	14.64	B	C
ATOM	11434	CD2	LEU	702	79.173	46.593	40.354	1.00	16.45	B	C
ATOM	11435	C	LEU	702	80.419	48.590	44.169	1.00	14.21	B	C
ATOM	11436	O	LEU	702	79.346	49.166	44.314	1.00	14.96	B	O
ATOM	11437	N	ILE	703	81.591	49.220	44.132	1.00	13.90	B	N
ATOM	11438	CA	ILE	703	81.737	50.662	44.294	1.00	13.91	B	C
ATOM	11439	CB	ILE	703	82.543	50.967	45.578	1.00	13.87	B	C
ATOM	11440	CG2	ILE	703	82.693	52.491	45.775	1.00	15.37	B	C
ATOM	11441	CG1	ILE	703	81.869	50.308	46.782	1.00	12.11	B	C
ATOM	11442	CD1	ILE	703	82.714	50.328	48.047	1.00	7.95	B	C
ATOM	11443	C	ILE	703	82.495	51.251	43.101	1.00	15.43	B	C
ATOM	11444	O	ILE	703	83.379	50.600	42.548	1.00	17.12	B	O
ATOM	11445	N	HIS	704	82.175	52.484	42.714	1.00	14.44	B	N
ATOM	11446	CA	HIS	704	82.866	53.098	41.579	1.00	14.11	B	C
ATOM	11447	CB	HIS	704	82.483	52.356	40.288	1.00	12.85	B	C
ATOM	11448	CG	HIS	704	83.539	52.386	39.224	1.00	13.44	B	C
ATOM	11449	CD2	HIS	704	84.363	53.377	38.806	1.00	12.54	B	C
ATOM	11450	ND1	HIS	704	83.827	51.293	38.435	1.00	12.00	B	N
ATOM	11451	CE1	HIS	704	84.782	51.607	37.578	1.00	10.09	B	C
ATOM	11452	NE2	HIS	704	85.125	52.865	37.782	1.00	12.68	B	N
ATOM	11453	C	HIS	704	82.533	54.584	41.457	1.00	13.37	B	C
ATOM	11454	O	HIS	704	81.420	55.007	41.770	1.00	15.67	B	O
ATOM	11455	N	GLY	705	83.513	55.372	41.027	1.00	10.99	B	N
ATOM	11456	CA	GLY	705	83.308	56.798	40.860	1.00	10.39	B	C
ATOM	11457	C	GLY	705	82.807	57.082	39.457	1.00	10.13	B	C
ATOM	11458	O	GLY	705	83.326	56.536	38.483	1.00	11.85	B	O
ATOM	11459	N	THR	706	81.805	57.942	39.347	1.00	10.36	B	N
ATOM	11460	CA	THR	706	81.215	58.272	38.054	1.00	9.96	B	C
ATOM	11461	CB	THR	706	79.935	59.072	38.232	1.00	6.56	B	C
ATOM	11462	OG1	THR	706	80.251	60.367	38.739	1.00	8.64	B	O
ATOM	11463	CG2	THR	706	79.025	58.372	39.215	1.00	8.26	B	C
ATOM	11464	C	THR	706	82.145	59.052	37.147	1.00	11.88	B	C
ATOM	11465	O	THR	706	81.994	59.018	35.927	1.00	13.83	B	O

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## FIG. 4 - 235

(Continued)

ATOM	11466	N	ALA	707	83.114	59.741	37.739	1.00	13.21	B	N
ATOM	11467	CA	ALA	707	84.075	60.522	36.969	1.00	14.57	B	C
ATOM	11468	CB	ALA	707	84.277	61.881	37.626	1.00	17.64	B	C
ATOM	11469	C	ALA	707	85.427	59.823	36.802	1.00	13.77	B	C
ATOM	11470	O	ALA	707	86.445	60.484	36.639	1.00	14.15	B	O
ATOM	11471	N	ASP	708	85.435	58.494	36.839	1.00	13.35	B	N
ATOM	11472	CA	ASP	708	86.667	57.721	36.685	1.00	12.65	B	C
ATOM	11473	CB	ASP	708	86.439	56.285	37.188	1.00	12.24	B	C
ATOM	11474	CG	ASP	708	87.737	55.536	37.453	1.00	10.05	B	C
ATOM	11475	OD1	ASP	708	88.738	55.775	36.749	1.00	11.19	B	O
ATOM	11476	OD2	ASP	708	87.751	54.686	38.362	1.00	9.31	B	O
ATOM	11477	C	ASP	708	87.091	57.696	35.202	1.00	13.18	B	C
ATOM	11478	O	ASP	708	86.475	57.023	34.368	1.00	13.78	B	O
ATOM	11479	N	ASP	709	88.156	58.423	34.891	1.00	12.80	B	N
ATOM	11480	CA	ASP	709	88.679	58.520	33.534	1.00	12.65	B	C
ATOM	11481	CB	ASP	709	89.442	59.825	33.397	1.00	11.74	B	C
ATOM	11482	CG	ASP	709	90.612	59.912	34.366	1.00	9.63	B	C
ATOM	11483	OD1	ASP	709	91.704	59.385	34.058	1.00	2.39	B	O
ATOM	11484	OD2	ASP	709	90.419	60.499	35.451	1.00	11.84	B	O
ATOM	11485	C	ASP	709	89.605	57.366	33.167	1.00	14.57	B	C
ATOM	11486	O	ASP	709	89.896	57.136	31.987	1.00	16.47	B	O
ATOM	11487	N	ASN	710	90.076	56.652	34.182	1.00	13.58	B	N
ATOM	11488	CA	ASN	710	90.981	55.524	33.990	1.00	13.56	B	C
ATOM	11489	CB	ASN	710	91.841	55.385	35.243	1.00	13.26	B	C
ATOM	11490	CG	ASN	710	92.987	54.440	35.059	1.00	12.07	B	C
ATOM	11491	OD1	ASN	710	93.951	54.478	35.821	1.00	16.69	B	O
ATOM	11492	ND2	ASN	710	92.898	53.578	34.058	1.00	8.28	B	N
ATOM	11493	C	ASN	710	90.177	54.236	33.724	1.00	14.26	B	C
ATOM	11494	O	ASN	710	90.142	53.737	32.598	1.00	14.29	B	O
ATOM	11495	N	VAL	711	89.560	53.692	34.773	1.00	13.24	B	N
ATOM	11496	CA	VAL	711	88.715	52.511	34.652	1.00	12.56	B	C
ATOM	11497	CB	VAL	711	88.835	51.585	35.868	1.00	11.72	B	C
ATOM	11498	CG1	VAL	711	88.048	50.311	35.624	1.00	7.36	B	C
ATOM	11499	CG2	VAL	711	90.287	51.274	36.141	1.00	13.94	B	C
ATOM	11500	C	VAL	711	87.315	53.119	34.645	1.00	14.01	B	C
ATOM	11501	O	VAL	711	86.768	53.471	35.694	1.00	13.52	B	O
ATOM	11502	N	HIS	712	86.746	53.249	33.456	1.00	13.66	B	N
ATOM	11503	CA	HIS	712	85.440	53.869	33.290	1.00	13.44	B	C
ATOM	11504	CB	HIS	712	85.132	53.956	31.794	1.00	12.94	B	C
ATOM	11505	CG	HIS	712	86.219	54.613	31.001	1.00	14.38	B	C
ATOM	11506	CD2	HIS	712	87.137	55.549	31.352	1.00	15.50	B	C
ATOM	11507	ND1	HIS	712	86.477	54.299	29.684	1.00	15.76	B	N
ATOM	11508	CE1	HIS	712	87.510	55.009	29.258	1.00	17.42	B	C
ATOM	11509	NE2	HIS	712	87.928	55.775	30.251	1.00	16.57	B	N
ATOM	11510	C	HIS	712	84.293	53.205	34.048	1.00	13.09	B	C
ATOM	11511	O	HIS	712	84.208	51.983	34.148	1.00	13.25	B	O
ATOM	11512	N	PHE	713	83.420	54.041	34.594	1.00	13.27	B	N
ATOM	11513	CA	PHE	713	82.253	53.586	35.335	1.00	15.36	B	C
ATOM	11514	CB	PHE	713	81.288	54.759	35.530	1.00	15.17	B	C

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ATOM	11515	CG	PHE	713	80.156	54.464	36.461	1.00	16.61	B	C
ATOM	11516	CD1	PHE	713	80.346	54.508	37.841	1.00	14.51	B	C
ATOM	11517	CD2	PHE	713	78.901	54.111	35.962	1.00	15.42	B	C
ATOM	11518	CE1	PHE	713	79.304	54.204	38.710	1.00	14.71	B	C
ATOM	11519	CE2	PHE	713	77.848	53.803	36.829	1.00	15.24	B	C
ATOM	11520	CZ	PHE	713	78.051	53.849	38.204	1.00	13.41	B	C
ATOM	11521	C	PHE	713	81.586	52.486	34.499	1.00	16.62	B	C
ATOM	11522	O	PHE	713	81.015	51.527	35.031	1.00	16.48	B	O
ATOM	11523	N	GLN	714	81.673	52.649	33.181	1.00	15.73	B	N
ATOM	11524	CA	GLN	714	81.121	51.699	32.228	1.00	16.08	B	C
ATOM	11525	CB	GLN	714	81.753	51.923	30.857	1.00	14.90	B	C
ATOM	11526	CG	GLN	714	81.699	50.703	29.946	1.00	16.13	B	C
ATOM	11527	CD	GLN	714	82.661	50.811	28.770	1.00	15.37	B	C
ATOM	11528	OE1	GLN	714	83.821	51.167	28.943	1.00	15.11	B	O
ATOM	11529	NE2	GLN	714	82.183	50.493	27.577	1.00	15.35	B	N
ATOM	11530	C	GLN	714	81.372	50.256	32.650	1.00	16.29	B	C
ATOM	11531	O	GLN	714	80.512	49.389	32.487	1.00	17.82	B	O
ATOM	11532	N	GLN	715	82.554	49.997	33.192	1.00	14.60	B	N
ATOM	11533	CA	GLN	715	82.900	48.646	33.593	1.00	14.55	B	C
ATOM	11534	CB	GLN	715	84.395	48.581	33.926	1.00	16.22	B	C
ATOM	11535	CG	GLN	715	85.270	49.086	32.767	1.00	16.01	B	C
ATOM	11536	CD	GLN	715	86.507	48.247	32.537	1.00	14.28	B	C
ATOM	11537	OE1	GLN	715	86.470	47.029	32.674	1.00	17.54	B	O
ATOM	11538	NE2	GLN	715	87.601	48.889	32.155	1.00	12.78	B	N
ATOM	11539	C	GLN	715	82.031	48.134	34.746	1.00	14.99	B	C
ATOM	11540	O	GLN	715	81.616	46.967	34.749	1.00	13.70	B	O
ATOM	11541	N	SER	716	81.742	49.002	35.714	1.00	12.14	B	N
ATOM	11542	CA	SER	716	80.893	48.602	36.829	1.00	11.18	B	C
ATOM	11543	CB	SER	716	81.057	49.544	38.028	1.00	11.19	B	C
ATOM	11544	OG	SER	716	82.278	49.295	38.700	1.00	13.48	B	O
ATOM	11545	C	SER	716	79.432	48.570	36.394	1.00	9.18	B	C
ATOM	11546	O	SER	716	78.682	47.692	36.814	1.00	5.81	B	O
ATOM	11547	N	ALA	717	79.026	49.517	35.552	1.00	8.69	B	N
ATOM	11548	CA	ALA	717	77.639	49.537	35.083	1.00	10.91	B	C
ATOM	11549	CB	ALA	717	77.400	50.708	34.143	1.00	10.07	B	C
ATOM	11550	C	ALA	717	77.304	48.219	34.382	1.00	10.72	B	C
ATOM	11551	O	ALA	717	76.212	47.696	34.539	1.00	14.08	B	O
ATOM	11552	N	GLN	718	78.252	47.682	33.623	1.00	10.89	B	N
ATOM	11553	CA	GLN	718	78.052	46.417	32.928	1.00	10.32	B	C
ATOM	11554	CB	GLN	718	79.137	46.224	31.858	1.00	8.83	B	C
ATOM	11555	CG	GLN	718	79.074	47.232	30.722	1.00	6.53	B	C
ATOM	11556	CD	GLN	718	78.002	46.900	29.691	1.00	8.70	B	C
ATOM	11557	OE1	GLN	718	76.970	46.319	30.012	1.00	13.43	B	O
ATOM	11558	NE2	GLN	718	78.243	47.278	28.449	1.00	11.12	B	N
ATOM	11559	C	GLN	718	78.056	45.235	33.908	1.00	10.68	B	C
ATOM	11560	O	GLN	718	77.357	44.248	33.695	1.00	13.48	B	O
ATOM	11561	N	ILE	719	78.834	45.320	34.981	1.00	12.24	B	N
ATOM	11562	CA	ILE	719	78.851	44.226	35.953	1.00	12.41	B	C
ATOM	11563	CB	ILE	719	79.892	44.434	37.079	1.00	12.88	B	C

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(Continued)

## FIG. 4 - 237

ATOM	11564	CG2	ILE	719	79.550	43.532	38.266	1.00	9.78	B	C
ATOM	11565	CG1	ILE	719	81.302	44.131	36.560	1.00	13.61	B	C
ATOM	11566	CD1	ILE	719	82.383	44.146	37.643	1.00	12.97	B	C
ATOM	11567	C	ILE	719	77.494	44.134	36.621	1.00	12.95	B	C
ATOM	11568	O	ILE	719	76.932	43.049	36.757	1.00	13.41	B	O
ATOM	11569	N	SER	720	76.979	45.286	37.043	1.00	12.96	B	N
ATOM	11570	CA	SER	720	75.694	45.345	37.716	1.00	13.07	B	C
ATOM	11571	CB	SER	720	75.418	46.771	38.211	1.00	12.56	B	C
ATOM	11572	OG	SER	720	75.435	47.716	37.147	1.00	15.69	B	O
ATOM	11573	C	SER	720	74.558	44.865	36.814	1.00	14.11	B	C
ATOM	11574	O	SER	720	73.712	44.073	37.238	1.00	13.45	B	O
ATOM	11575	N	LYS	721	74.536	45.329	35.569	1.00	12.91	B	N
ATOM	11576	CA	LYS	721	73.474	44.919	34.664	1.00	14.31	B	C
ATOM	11577	CB	LYS	721	73.647	45.596	33.303	1.00	14.17	B	C
ATOM	11578	CG	LYS	721	72.613	45.188	32.264	1.00	10.06	B	C
ATOM	11579	CD	LYS	721	72.241	46.368	31.378	1.00	10.77	B	C
ATOM	11580	CE	LYS	721	73.427	46.932	30.611	1.00	9.97	B	C
ATOM	11581	NZ	LYS	721	73.939	45.970	29.595	1.00	11.67	B	N
ATOM	11582	C	LYS	721	73.431	43.396	34.504	1.00	15.75	B	C
ATOM	11583	O	LYS	721	72.349	42.803	34.403	1.00	14.39	B	O
ATOM	11584	N	ALA	722	74.605	42.766	34.501	1.00	14.45	B	N
ATOM	11585	CA	ALA	722	74.684	41.320	34.353	1.00	13.03	B	C
ATOM	11586	CB	ALA	722	76.137	40.889	34.146	1.00	11.46	B	C
ATOM	11587	C	ALA	722	74.083	40.607	35.564	1.00	14.14	B	C
ATOM	11588	O	ALA	722	73.369	39.606	35.417	1.00	14.70	B	O
ATOM	11589	N	LEU	723	74.358	41.124	36.758	1.00	13.91	B	N
ATOM	11590	CA	LEU	723	73.832	40.520	37.974	1.00	15.06	B	C
ATOM	11591	CB	LEU	723	74.442	41.184	39.204	1.00	16.63	B	C
ATOM	11592	CG	LEU	723	75.957	40.999	39.306	1.00	16.43	B	C
ATOM	11593	CD1	LEU	723	76.504	41.863	40.415	1.00	18.97	B	C
ATOM	11594	CD2	LEU	723	76.280	39.535	39.546	1.00	15.22	B	C
ATOM	11595	C	LEU	723	72.323	40.668	37.980	1.00	16.46	B	C
ATOM	11596	O	LEU	723	71.586	39.731	38.310	1.00	18.39	B	O
ATOM	11597	N	VAL	724	71.858	41.849	37.604	1.00	16.97	B	N
ATOM	11598	CA	VAL	724	70.429	42.079	37.533	1.00	17.76	B	C
ATOM	11599	CB	VAL	724	70.126	43.526	37.084	1.00	17.79	B	C
ATOM	11600	CG1	VAL	724	68.660	43.678	36.728	1.00	18.59	B	C
ATOM	11601	CG2	VAL	724	70.479	44.487	38.213	1.00	19.61	B	C
ATOM	11602	C	VAL	724	69.844	41.079	36.532	1.00	18.06	B	C
ATOM	11603	O	VAL	724	68.824	40.441	36.800	1.00	16.03	B	O
ATOM	11604	N	ASP	725	70.509	40.920	35.391	1.00	19.41	B	N
ATOM	11605	CA	ASP	725	70.015	39.999	34.379	1.00	21.58	B	C
ATOM	11606	CB	ASP	725	70.965	39.930	33.191	1.00	23.71	B	C
ATOM	11607	CG	ASP	725	70.957	41.197	32.372	1.00	27.35	B	C
ATOM	11608	OD1	ASP	725	69.919	41.895	32.368	1.00	27.29	B	O
ATOM	11609	OD2	ASP	725	71.983	41.486	31.717	1.00	31.72	B	O
ATOM	11610	C	ASP	725	69.748	38.591	34.893	1.00	22.63	B	C
ATOM	11611	O	ASP	725	68.763	37.974	34.474	1.00	24.48	B	O
ATOM	11612	N	VAL	726	70.607	38.075	35.781	1.00	20.53	B	N

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## FIG. 4 - 238

ATOM	11613	CA	VAL	726	70.409	36.726	36.329	1.00	17.93	B	C
ATOM	11614	CB	VAL	726	71.727	35.920	36.392	1.00	19.28	B	C
ATOM	11615	CG1	VAL	726	72.246	35.672	34.994	1.00	19.33	B	C
ATOM	11616	CG2	VAL	726	72.763	36.660	37.238	1.00	19.80	B	C
ATOM	11617	C	VAL	726	69.789	36.741	37.723	1.00	17.35	B	C
ATOM	11618	O	VAL	726	69.858	35.756	38.463	1.00	16.63	B	O
ATOM	11619	N	GLY	727	69.198	37.875	38.081	1.00	17.14	B	N
ATOM	11620	CA	GLY	727	68.548	38.012	39.370	1.00	15.42	B	C
ATOM	11621	C	GLY	727	69.387	37.856	40.626	1.00	15.90	B	C
ATOM	11622	O	GLY	727	68.961	37.182	41.559	1.00	17.97	B	O
ATOM	11623	N	VAL	728	70.568	38.462	40.675	1.00	15.07	B	N
ATOM	11624	CA	VAL	728	71.389	38.357	41.876	1.00	14.10	B	C
ATOM	11625	CB	VAL	728	72.859	37.972	41.574	1.00	14.97	B	C
ATOM	11626	CG1	VAL	728	73.693	38.145	42.829	1.00	13.51	B	C
ATOM	11627	CG2	VAL	728	72.954	36.514	41.109	1.00	15.40	B	C
ATOM	11628	C	VAL	728	71.396	39.687	42.603	1.00	14.73	B	C
ATOM	11629	O	VAL	728	71.738	40.714	42.025	1.00	14.56	B	O
ATOM	11630	N	ASP	729	71.007	39.672	43.872	1.00	15.13	B	N
ATOM	11631	CA	ASP	729	70.998	40.896	44.646	1.00	15.32	B	C
ATOM	11632	CB	ASP	729	70.146	40.731	45.903	1.00	15.31	B	C
ATOM	11633	CG	ASP	729	70.034	42.019	46.696	1.00	18.11	B	C
ATOM	11634	OD1	ASP	729	69.663	43.055	46.104	1.00	20.57	B	O
ATOM	11635	OD2	ASP	729	70.317	42.011	47.907	1.00	20.06	B	O
ATOM	11636	C	ASP	729	72.441	41.185	45.021	1.00	16.27	B	C
ATOM	11637	O	ASP	729	73.253	40.270	45.117	1.00	17.70	B	O
ATOM	11638	N	PHE	730	72.772	42.454	45.211	1.00	16.74	B	N
ATOM	11639	CA	PHE	730	74.136	42.824	45.579	1.00	16.43	B	C
ATOM	11640	CB	PHE	730	75.061	42.734	44.361	1.00	13.47	B	C
ATOM	11641	CG	PHE	730	74.744	43.728	43.304	1.00	12.81	B	C
ATOM	11642	CD1	PHE	730	75.282	45.006	43.355	1.00	12.64	B	C
ATOM	11643	CD2	PHE	730	73.828	43.423	42.303	1.00	12.46	B	C
ATOM	11644	CE1	PHE	730	74.907	45.966	42.432	1.00	11.61	B	C
ATOM	11645	CE2	PHE	730	73.446	44.377	41.376	1.00	9.11	B	C
ATOM	11646	CZ	PHE	730	73.986	45.653	41.443	1.00	10.39	B	C
ATOM	11647	C	PHE	730	74.112	44.242	46.114	1.00	17.87	B	C
ATOM	11648	O	PHE	730	73.094	44.928	46.014	1.00	19.72	B	O
ATOM	11649	N	GLN	731	75.230	44.673	46.689	1.00	18.41	B	N
ATOM	11650	CA	GLN	731	75.344	46.015	47.246	1.00	17.25	B	C
ATOM	11651	CB	GLN	731	76.089	45.961	48.569	1.00	18.02	B	C
ATOM	11652	CG	GLN	731	75.547	44.948	49.536	1.00	25.59	B	C
ATOM	11653	CD	GLN	731	74.087	45.183	49.854	1.00	29.48	B	C
ATOM	11654	OE1	GLN	731	73.699	46.275	50.281	1.00	31.32	B	O
ATOM	11655	NE2	GLN	731	73.263	44.157	49.647	1.00	32.13	B	N
ATOM	11656	C	GLN	731	76.124	46.889	46.272	1.00	16.69	B	C
ATOM	11657	O	GLN	731	77.060	46.417	45.623	1.00	13.71	B	O
ATOM	11658	N	ALA	732	75.737	48.158	46.172	1.00	15.59	B	N
ATOM	11659	CA	ALA	732	76.425	49.084	45.284	1.00	15.79	B	C
ATOM	11660	CB	ALA	732	75.718	49.147	43.946	1.00	15.47	B	C
ATOM	11661	C	ALA	732	76.540	50.486	45.867	1.00	17.21	B	C

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(Continued)

## FIG. 4 - 239

ATOM	11662	O	ALA	732	75.769	50.897	46.734	1.00	17.93	B	O
ATOM	11663	N	MET	733	77.528	51.220	45.382	1.00	17.27	B	N
ATOM	11664	CA	MET	733	77.737	52.587	45.812	1.00	17.39	B	C
ATOM	11665	CB	MET	733	78.500	52.628	47.136	1.00	18.98	B	C
ATOM	11666	CG	MET	733	78.775	54.028	47.661	1.00	18.20	B	C
ATOM	11667	SD	MET	733	77.278	54.979	47.988	1.00	21.42	B	S
ATOM	11668	CE	MET	733	76.781	54.324	49.578	1.00	19.12	B	C
ATOM	11669	C	MET	733	78.539	53.268	44.719	1.00	17.47	B	C
ATOM	11670	O	MET	733	79.604	52.783	44.318	1.00	17.30	B	O
ATOM	11671	N	TRP	734	78.007	54.378	44.220	1.00	16.37	B	N
ATOM	11672	CA	TRP	734	78.673	55.147	43.175	1.00	15.48	B	C
ATOM	11673	CB	TRP	734	77.685	55.428	42.033	1.00	14.82	B	C
ATOM	11674	CG	TRP	734	76.691	56.523	42.353	1.00	14.06	B	C
ATOM	11675	CD2	TRP	734	75.299	56.363	42.650	1.00	12.49	B	C
ATOM	11676	CE2	TRP	734	74.785	57.645	42.939	1.00	12.15	B	C
ATOM	11677	CE3	TRP	734	74.437	55.259	42.701	1.00	12.01	B	C
ATOM	11678	CD1	TRP	734	76.953	57.857	42.468	1.00	12.61	B	C
ATOM	11679	NE1	TRP	734	75.817	58.535	42.821	1.00	13.60	B	N
ATOM	11680	CZ2	TRP	734	73.449	57.858	43.276	1.00	11.75	B	C
ATOM	11681	CZ3	TRP	734	73.115	55.466	43.034	1.00	13.39	B	C
ATOM	11682	CH2	TRP	734	72.629	56.762	43.319	1.00	13.13	B	C
ATOM	11683	C	TRP	734	79.111	56.457	43.831	1.00	13.60	B	C
ATOM	11684	O	TRP	734	78.491	56.881	44.788	1.00	14.71	B	O
ATOM	11685	N	TYR	735	80.174	57.090	43.346	1.00	13.31	B	N
ATOM	11686	CA	TYR	735	80.598	58.366	43.926	1.00	12.17	B	C
ATOM	11687	CB	TYR	735	81.990	58.260	44.575	1.00	10.49	B	C
ATOM	11688	CG	TYR	735	81.964	57.577	45.920	1.00	10.18	B	C
ATOM	11689	CD1	TYR	735	81.464	58.232	47.045	1.00	11.23	B	C
ATOM	11690	CE1	TYR	735	81.321	57.567	48.272	1.00	11.72	B	C
ATOM	11691	CD2	TYR	735	82.336	56.241	46.052	1.00	11.30	B	C
ATOM	11692	CE2	TYR	735	82.198	55.567	47.270	1.00	11.75	B	C
ATOM	11693	CZ	TYR	735	81.687	56.235	48.372	1.00	12.02	B	C
ATOM	11694	OH	TYR	735	81.511	55.564	49.563	1.00	13.79	B	O
ATOM	11695	C	TYR	735	80.595	59.430	42.845	1.00	14.20	B	C
ATOM	11696	O	TYR	735	81.391	59.393	41.910	1.00	15.56	B	O
ATOM	11697	N	THR	736	79.669	60.372	42.977	1.00	15.66	B	N
ATOM	11698	CA	THR	736	79.517	61.459	42.026	1.00	14.01	B	C
ATOM	11699	CB	THR	736	78.395	62.401	42.469	1.00	13.01	B	C
ATOM	11700	OG1	THR	736	77.163	61.673	42.534	1.00	13.00	B	O
ATOM	11701	CG2	THR	736	78.256	63.571	41.503	1.00	11.91	B	C
ATOM	11702	C	THR	736	80.789	62.278	41.882	1.00	16.80	B	C
ATOM	11703	O	THR	736	81.357	62.730	42.875	1.00	19.71	B	O
ATOM	11704	N	ASP	737	81.230	62.457	40.640	1.00	16.82	B	N
ATOM	11705	CA	ASP	737	82.407	63.257	40.322	1.00	15.22	B	C
ATOM	11706	CB	ASP	737	82.151	64.728	40.684	1.00	15.24	B	C
ATOM	11707	CG	ASP	737	81.101	65.380	39.785	1.00	17.61	B	C
ATOM	11708	OD1	ASP	737	80.697	64.753	38.779	1.00	16.59	B	O
ATOM	11709	OD2	ASP	737	80.680	66.525	40.078	1.00	19.23	B	O
ATOM	11710	C	ASP	737	83.737	62.811	40.912	1.00	15.17	B	C

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(Continued)

## FIG. 4 - 240

ATOM	11711	O	ASP	737	84.716	63.560	40.882	1.00	14.33	B	O
ATOM	11712	N	GLU	738	83.790	61.603	41.453	1.00	14.73	B	N
ATOM	11713	CA	GLU	738	85.054	61.112	41.986	1.00	14.51	B	C
ATOM	11714	CB	GLU	738	84.829	60.208	43.206	1.00	15.23	B	C
ATOM	11715	CG	GLU	738	84.353	60.935	44.448	1.00	16.91	B	C
ATOM	11716	CD	GLU	738	85.355	61.958	44.956	1.00	19.02	B	C
ATOM	11717	OE1	GLU	738	86.513	61.580	45.222	1.00	19.93	B	O
ATOM	11718	OE2	GLU	738	84.985	63.142	45.100	1.00	19.97	B	O
ATOM	11719	C	GLU	738	85.718	60.319	40.867	1.00	13.36	B	C
ATOM	11720	O	GLU	738	85.037	59.763	40.005	1.00	13.24	B	O
ATOM	11721	N	ASP	739	87.042	60.275	40.858	1.00	12.47	B	N
ATOM	11722	CA	ASP	739	87.716	59.522	39.824	1.00	12.05	B	C
ATOM	11723	CB	ASP	739	88.809	60.369	39.166	1.00	12.46	B	C
ATOM	11724	CG	ASP	739	89.952	60.717	40.101	1.00	16.27	B	C
ATOM	11725	OD1	ASP	739	90.706	61.653	39.751	1.00	16.93	B	O
ATOM	11726	OD2	ASP	739	90.116	60.066	41.158	1.00	16.75	B	O
ATOM	11727	C	ASP	739	88.248	58.187	40.351	1.00	13.65	B	C
ATOM	11728	O	ASP	739	87.781	57.686	41.372	1.00	14.63	B	O
ATOM	11729	N	HIS	740	89.217	57.609	39.661	1.00	12.45	B	N
ATOM	11730	CA	HIS	740	89.735	56.311	40.041	1.00	12.91	B	C
ATOM	11731	CB	HIS	740	90.795	55.872	39.035	1.00	12.28	B	C
ATOM	11732	CG	HIS	740	91.112	54.418	39.105	1.00	12.12	B	C
ATOM	11733	CD2	HIS	740	92.292	53.763	39.179	1.00	12.56	B	C
ATOM	11734	ND1	HIS	740	90.133	53.449	39.081	1.00	12.00	B	N
ATOM	11735	CE1	HIS	740	90.697	52.256	39.136	1.00	11.97	B	C
ATOM	11736	NE2	HIS	740	92.006	52.419	39.194	1.00	12.98	B	N
ATOM	11737	C	HIS	740	90.298	56.209	41.447	1.00	14.77	B	C
ATOM	11738	O	HIS	740	90.302	55.133	42.041	1.00	16.10	B	O
ATOM	11739	N	GLY	741	90.775	57.320	41.986	1.00	14.45	B	N
ATOM	11740	CA	GLY	741	91.345	57.271	43.311	1.00	13.32	B	C
ATOM	11741	C	GLY	741	90.381	57.572	44.431	1.00	14.78	B	C
ATOM	11742	O	GLY	741	90.763	57.445	45.590	1.00	16.71	B	O
ATOM	11743	N	ILE	742	89.144	57.946	44.103	1.00	14.08	B	N
ATOM	11744	CA	ILE	742	88.146	58.298	45.111	1.00	14.39	B	C
ATOM	11745	CB	ILE	742	87.309	57.082	45.520	1.00	14.12	B	C
ATOM	11746	CG2	ILE	742	86.121	57.539	46.345	1.00	13.12	B	C
ATOM	11747	CG1	ILE	742	86.830	56.336	44.273	1.00	13.94	B	C
ATOM	11748	CD1	ILE	742	85.833	55.214	44.553	1.00	10.86	B	C
ATOM	11749	C	ILE	742	88.892	58.827	46.335	1.00	15.89	B	C
ATOM	11750	O	ILE	742	88.706	58.350	47.453	1.00	17.67	B	O
ATOM	11751	N	ALA	743	89.737	59.828	46.108	1.00	16.48	B	N
ATOM	11752	CA	ALA	743	90.570	60.381	47.157	1.00	15.34	B	C
ATOM	11753	CB	ALA	743	91.985	60.508	46.651	1.00	16.86	B	C
ATOM	11754	C	ALA	743	90.149	61.689	47.779	1.00	16.53	B	C
ATOM	11755	O	ALA	743	90.809	62.153	48.711	1.00	18.69	B	O
ATOM	11756	N	SER	744	89.088	62.312	47.287	1.00	14.28	B	N
ATOM	11757	CA	SER	744	88.681	63.556	47.908	1.00	14.62	B	C
ATOM	11758	CB	SER	744	87.369	64.059	47.321	1.00	16.50	B	C
ATOM	11759	OG	SER	744	86.314	63.152	47.573	1.00	22.09	B	O

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(Continued)

## FIG. 4 - 241

ATOM	11760	C	SER	744	88.515	63.251	49.390	1.00	15.05	B	C
ATOM	11761	O	SER	744	88.136	62.147	49.770	1.00	17.03	B	O
ATOM	11762	N	SER	745	88.822	64.223	50.229	1.00	16.05	B	N
ATOM	11763	CA	SER	745	88.712	64.051	51.666	1.00	15.38	B	C
ATOM	11764	CB	SER	745	88.811	65.410	52.361	1.00	15.23	B	C
ATOM	11765	OG	SER	745	88.357	65.318	53.698	1.00	20.36	B	O
ATOM	11766	C	SER	745	87.427	63.360	52.103	1.00	14.58	B	C
ATOM	11767	O	SER	745	87.467	62.334	52.773	1.00	15.64	B	O
ATOM	11768	N	THR	746	86.287	63.925	51.728	1.00	13.39	B	N
ATOM	11769	CA	THR	746	85.009	63.355	52.121	1.00	12.46	B	C
ATOM	11770	CB	THR	746	83.836	64.299	51.755	1.00	13.02	B	C
ATOM	11771	OG1	THR	746	83.858	64.579	50.347	1.00	12.13	B	O
ATOM	11772	CG2	THR	746	83.929	65.599	52.547	1.00	6.36	B	C
ATOM	11773	C	THR	746	84.748	61.982	51.513	1.00	13.71	B	C
ATOM	11774	O	THR	746	84.382	61.045	52.215	1.00	13.77	B	O
ATOM	11775	N	ALA	747	84.948	61.852	50.211	1.00	15.70	B	N
ATOM	11776	CA	ALA	747	84.698	60.575	49.556	1.00	17.75	B	C
ATOM	11777	CB	ALA	747	84.918	60.698	48.047	1.00	18.85	B	C
ATOM	11778	C	ALA	747	85.579	59.482	50.133	1.00	16.94	B	C
ATOM	11779	O	ALA	747	85.136	58.344	50.314	1.00	17.92	B	O
ATOM	11780	N	HIS	748	86.828	59.829	50.418	1.00	15.98	B	N
ATOM	11781	CA	HIS	748	87.772	58.873	50.987	1.00	15.53	B	C
ATOM	11782	CB	HIS	748	89.130	59.547	51.194	1.00	14.50	B	C
ATOM	11783	CG	HIS	748	90.106	58.721	51.974	1.00	12.65	B	C
ATOM	11784	CD2	HIS	748	90.772	58.979	53.124	1.00	12.46	B	C
ATOM	11785	ND1	HIS	748	90.517	57.472	51.566	1.00	11.91	B	N
ATOM	11786	CE1	HIS	748	91.397	56.998	52.430	1.00	12.20	B	C
ATOM	11787	NE2	HIS	748	91.569	57.893	53.384	1.00	9.44	B	N
ATOM	11788	C	HIS	748	87.259	58.310	52.316	1.00	15.00	B	C
ATOM	11789	O	HIS	748	87.272	57.097	52.533	1.00	14.52	B	O
ATOM	11790	N	GLN	749	86.808	59.196	53.200	1.00	14.63	B	N
ATOM	11791	CA	GLN	749	86.283	58.780	54.496	1.00	15.23	B	C
ATOM	11792	CB	GLN	749	86.045	59.999	55.378	1.00	15.87	B	C
ATOM	11793	CG	GLN	749	87.314	60.722	55.740	1.00	22.62	B	C
ATOM	11794	CD	GLN	749	87.056	61.956	56.564	1.00	25.83	B	C
ATOM	11795	OE1	GLN	749	86.511	61.873	57.664	1.00	29.51	B	O
ATOM	11796	NE2	GLN	749	87.443	63.116	56.039	1.00	27.64	B	N
ATOM	11797	C	GLN	749	84.984	57.999	54.348	1.00	14.70	B	C
ATOM	11798	O	GLN	749	84.749	57.015	55.054	1.00	14.10	B	O
ATOM	11799	N	HIS	750	84.147	58.440	53.415	1.00	13.44	B	N
ATOM	11800	CA	HIS	750	82.865	57.808	53.174	1.00	12.63	B	C
ATOM	11801	CB	HIS	750	82.021	58.685	52.247	1.00	13.59	B	C
ATOM	11802	CG	HIS	750	80.587	58.272	52.176	1.00	12.41	B	C
ATOM	11803	CD2	HIS	750	79.475	58.823	52.713	1.00	13.33	B	C
ATOM	11804	ND1	HIS	750	80.175	57.128	51.530	1.00	12.98	B	N
ATOM	11805	CE1	HIS	750	78.869	56.992	51.673	1.00	14.44	B	C
ATOM	11806	NE2	HIS	750	78.419	58.007	52.386	1.00	13.43	B	N
ATOM	11807	C	HIS	750	82.985	56.404	52.595	1.00	13.84	B	C
ATOM	11808	O	HIS	750	82.265	55.499	53.011	1.00	14.53	B	O

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(Continued)

## FIG. 4 - 242

ATOM	11809	N	ILE	751	83.885	56.203	51.638	1.00	13.03	B	N
ATOM	11810	CA	ILE	751	84.013	54.875	51.077	1.00	12.47	B	C
ATOM	11811	CB	ILE	751	84.927	54.838	49.814	1.00	13.01	B	C
ATOM	11812	CG2	ILE	751	86.326	55.361	50.137	1.00	12.55	B	C
ATOM	11813	CG1	ILE	751	84.999	53.395	49.287	1.00	12.09	B	C
ATOM	11814	CD1	ILE	751	85.677	53.240	47.939	1.00	11.16	B	C
ATOM	11815	C	ILE	751	84.546	53.893	52.111	1.00	12.65	B	C
ATOM	11816	O	ILE	751	84.025	52.790	52.241	1.00	12.49	B	O
ATOM	11817	N	TYR	752	85.575	54.284	52.858	1.00	13.74	B	N
ATOM	11818	CA	TYR	752	86.137	53.364	53.850	1.00	14.04	B	C
ATOM	11819	CB	TYR	752	87.486	53.883	54.379	1.00	11.26	B	C
ATOM	11820	CG	TYR	752	88.628	53.468	53.472	1.00	9.86	B	C
ATOM	11821	CD1	TYR	752	89.037	52.132	53.408	1.00	10.53	B	C
ATOM	11822	CE1	TYR	752	90.015	51.712	52.502	1.00	9.48	B	C
ATOM	11823	CD2	TYR	752	89.235	54.383	52.608	1.00	9.66	B	C
ATOM	11824	CE2	TYR	752	90.219	53.974	51.692	1.00	8.36	B	C
ATOM	11825	CZ	TYR	752	90.597	52.639	51.646	1.00	9.94	B	C
ATOM	11826	OH	TYR	752	91.536	52.223	50.739	1.00	10.79	B	O
ATOM	11827	C	TYR	752	85.170	53.067	54.973	1.00	13.42	B	C
ATOM	11828	O	TYR	752	85.176	51.972	55.524	1.00	13.56	B	O
ATOM	11829	N	THR	753	84.323	54.040	55.295	1.00	14.48	B	N
ATOM	11830	CA	THR	753	83.316	53.864	56.330	1.00	14.27	B	C
ATOM	11831	CB	THR	753	82.582	55.187	56.618	1.00	13.68	B	C
ATOM	11832	OG1	THR	753	83.519	56.136	57.130	1.00	17.48	B	O
ATOM	11833	CG2	THR	753	81.459	54.987	57.629	1.00	7.20	B	C
ATOM	11834	C	THR	753	82.301	52.849	55.815	1.00	16.15	B	C
ATOM	11835	O	THR	753	81.958	51.894	56.508	1.00	18.93	B	O
ATOM	11836	N	HIS	754	81.830	53.056	54.589	1.00	15.38	B	N
ATOM	11837	CA	HIS	754	80.840	52.163	53.999	1.00	16.06	B	C
ATOM	11838	CB	HIS	754	80.424	52.666	52.620	1.00	15.26	B	C
ATOM	11839	CG	HIS	754	79.109	52.128	52.162	1.00	16.39	B	C
ATOM	11840	CD2	HIS	754	78.779	51.362	51.095	1.00	15.75	B	C
ATOM	11841	ND1	HIS	754	77.936	52.353	52.850	1.00	17.30	B	N
ATOM	11842	CE1	HIS	754	76.940	51.750	52.228	1.00	15.86	B	C
ATOM	11843	NE2	HIS	754	77.425	51.141	51.161	1.00	17.13	B	N
ATOM	11844	C	HIS	754	81.349	50.731	53.886	1.00	16.28	B	C
ATOM	11845	O	HIS	754	80.639	49.788	54.238	1.00	17.31	B	O
ATOM	11846	N	MET	755	82.571	50.564	53.383	1.00	15.98	B	N
ATOM	11847	CA	MET	755	83.158	49.234	53.250	1.00	16.05	B	C
ATOM	11848	CB	MET	755	84.532	49.300	52.573	1.00	15.41	B	C
ATOM	11849	CG	MET	755	84.491	49.542	51.081	1.00	17.11	B	C
ATOM	11850	SD	MET	755	86.112	49.308	50.322	1.00	18.41	B	S
ATOM	11851	CE	MET	755	86.882	50.855	50.742	1.00	20.74	B	C
ATOM	11852	C	MET	755	83.309	48.582	54.623	1.00	15.38	B	C
ATOM	11853	O	MET	755	83.080	47.390	54.783	1.00	13.30	B	O
ATOM	11854	N	SER	756	83.701	49.371	55.614	1.00	15.36	B	N
ATOM	11855	CA	SER	756	83.854	48.833	56.946	1.00	18.52	B	C
ATOM	11856	CB	SER	756	84.413	49.903	57.878	1.00	18.88	B	C
ATOM	11857	OG	SER	756	85.723	50.257	57.477	1.00	18.74	B	O

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(Continued)

## FIG. 4 - 243

ATOM	11858	C	SER	756	82.515	48.282	57.462	1.00	19.14	B	C
ATOM	11859	O	SER	756	82.464	47.158	57.975	1.00	19.94	B	O
ATOM	11860	N	HIS	757	81.435	49.048	57.324	1.00	17.68	B	N
ATOM	11861	CA	HIS	757	80.134	48.549	57.770	1.00	19.20	B	C
ATOM	11862	CB	HIS	757	78.990	49.486	57.371	1.00	18.83	B	C
ATOM	11863	CG	HIS	757	78.983	50.794	58.095	1.00	21.13	B	C
ATOM	11864	CD2	HIS	757	78.697	52.046	57.666	1.00	22.10	B	C
ATOM	11865	ND1	HIS	757	79.230	50.899	59.447	1.00	22.62	B	N
ATOM	11866	CE1	HIS	757	79.096	52.159	59.820	1.00	23.60	B	C
ATOM	11867	NE2	HIS	757	78.772	52.876	58.758	1.00	24.81	B	N
ATOM	11868	C	HIS	757	79.866	47.190	57.120	1.00	17.94	B	C
ATOM	11869	O	HIS	757	79.416	46.251	57.772	1.00	16.58	B	O
ATOM	11870	N	PHE	758	80.158	47.103	55.828	1.00	17.93	B	N
ATOM	11871	CA	PHE	758	79.926	45.888	55.052	1.00	18.80	B	C
ATOM	11872	CB	PHE	758	80.286	46.138	53.586	1.00	15.70	B	C
ATOM	11873	CG	PHE	758	79.952	44.997	52.677	1.00	10.77	B	C
ATOM	11874	CD1	PHE	758	78.646	44.790	52.251	1.00	8.39	B	C
ATOM	11875	CD2	PHE	758	80.941	44.120	52.254	1.00	6.53	B	C
ATOM	11876	CE1	PHE	758	78.334	43.716	51.409	1.00	9.32	B	C
ATOM	11877	CE2	PHE	758	80.638	43.045	51.417	1.00	6.01	B	C
ATOM	11878	CZ	PHE	758	79.340	42.836	50.991	1.00	2.78	B	C
ATOM	11879	C	PHE	758	80.697	44.674	55.560	1.00	20.68	B	C
ATOM	11880	O	PHE	758	80.110	43.631	55.851	1.00	21.00	B	O
ATOM	11881	N	ILE	759	82.014	44.811	55.654	1.00	23.57	B	N
ATOM	11882	CA	ILE	759	82.858	43.722	56.117	1.00	25.05	B	C
ATOM	11883	CB	ILE	759	84.364	44.129	56.069	1.00	25.44	B	C
ATOM	11884	CG2	ILE	759	84.994	44.041	57.437	1.00	28.98	B	C
ATOM	11885	CG1	ILE	759	85.128	43.189	55.142	1.00	26.52	B	C
ATOM	11886	CD1	ILE	759	84.706	43.263	53.704	1.00	26.84	B	C
ATOM	11887	C	ILE	759	82.441	43.318	57.529	1.00	25.34	B	C
ATOM	11888	O	ILE	759	82.420	42.136	57.866	1.00	25.50	B	O
ATOM	11889	N	LYS	760	82.081	44.299	58.346	1.00	26.11	B	N
ATOM	11890	CA	LYS	760	81.671	44.012	59.713	1.00	26.62	B	C
ATOM	11891	CB	LYS	760	81.444	45.300	60.487	1.00	26.43	B	C
ATOM	11892	CG	LYS	760	82.178	45.298	61.792	1.00	29.00	B	C
ATOM	11893	CD	LYS	760	83.666	45.271	61.537	1.00	28.96	B	C
ATOM	11894	CE	LYS	760	84.139	46.665	61.250	1.00	30.01	B	C
ATOM	11895	NZ	LYS	760	83.776	47.523	62.420	1.00	31.29	B	N
ATOM	11896	C	LYS	760	80.406	43.179	59.740	1.00	27.08	B	C
ATOM	11897	O	LYS	760	80.312	42.200	60.473	1.00	28.46	B	O
ATOM	11898	N	GLN	761	79.431	43.581	58.940	1.00	28.08	B	N
ATOM	11899	CA	GLN	761	78.170	42.866	58.844	1.00	29.69	B	C
ATOM	11900	CB	GLN	761	77.213	43.652	57.942	1.00	31.26	B	C
ATOM	11901	CG	GLN	761	76.072	42.855	57.347	1.00	34.99	B	C
ATOM	11902	CD	GLN	761	76.477	42.140	56.072	1.00	37.85	B	C
ATOM	11903	OE1	GLN	761	76.800	42.775	55.062	1.00	37.29	B	O
ATOM	11904	NE2	GLN	761	76.464	40.808	56.112	1.00	39.80	B	N
ATOM	11905	C	GLN	761	78.401	41.456	58.295	1.00	30.00	B	C
ATOM	11906	O	GLN	761	77.791	40.494	58.753	1.00	31.14	B	O

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(Continued)

## FIG. 4 - 244

ATOM	11907	N	CYS	762	79.291	41.333	57.320	1.00	29.71	B	N
ATOM	11908	CA	CYS	762	79.588	40.035	56.731	1.00	30.30	B	C
ATOM	11909	C	CYS	762	80.275	39.077	57.712	1.00	30.21	B	C
ATOM	11910	O	CYS	762	80.153	37.860	57.578	1.00	29.67	B	O
ATOM	11911	CB	CYS	762	80.458	40.212	55.474	1.00	30.01	B	C
ATOM	11912	SG	CYS	762	81.198	38.665	54.849	1.00	33.72	B	S
ATOM	11913	N	PHE	763	80.986	39.618	58.698	1.00	30.53	B	N
ATOM	11914	CA	PHE	763	81.694	38.783	59.664	1.00	31.28	B	C
ATOM	11915	CB	PHE	763	83.112	39.310	59.885	1.00	29.29	B	C
ATOM	11916	CG	PHE	763	84.052	39.057	58.736	1.00	27.21	B	C
ATOM	11917	CD1	PHE	763	83.663	38.280	57.650	1.00	26.19	B	C
ATOM	11918	CD2	PHE	763	85.348	39.572	58.762	1.00	26.38	B	C
ATOM	11919	CE1	PHE	763	84.552	38.015	56.605	1.00	27.91	B	C
ATOM	11920	CE2	PHE	763	86.249	39.316	57.727	1.00	27.36	B	C
ATOM	11921	CZ	PHE	763	85.851	38.533	56.643	1.00	27.55	B	C
ATOM	11922	C	PHE	763	80.994	38.666	61.011	1.00	34.52	B	C
ATOM	11923	O	PHE	763	81.473	37.970	61.908	1.00	32.78	B	O
ATOM	11924	N	SER	764	79.862	39.346	61.151	1.00	39.49	B	N
ATOM	11925	CA	SER	764	79.099	39.319	62.393	1.00	43.60	B	C
ATOM	11926	CB	SER	764	77.860	40.199	62.273	1.00	44.56	B	C
ATOM	11927	OG	SER	764	78.218	41.528	61.948	1.00	50.05	B	O
ATOM	11928	C	SER	764	78.668	37.909	62.746	1.00	45.96	B	C
ATOM	11929	O	SER	764	77.885	37.289	62.028	1.00	45.86	B	O
ATOM	11930	N	LEU	765	79.189	37.404	63.856	1.00	49.22	B	N
ATOM	11931	CA	LEU	765	78.845	36.070	64.317	1.00	52.03	B	C
ATOM	11932	CB	LEU	765	79.754	35.678	65.481	1.00	52.53	B	C
ATOM	11933	CG	LEU	765	81.234	35.558	65.115	1.00	52.85	B	C
ATOM	11934	CD1	LEU	765	82.074	35.452	66.376	1.00	53.55	B	C
ATOM	11935	CD2	LEU	765	81.435	34.344	64.214	1.00	52.54	B	C
ATOM	11936	C	LEU	765	77.383	36.069	64.761	1.00	54.34	B	C
ATOM	11937	O	LEU	765	77.019	36.721	65.743	1.00	53.63	B	O
ATOM	11938	N	PRO	766	76.523	35.340	64.031	1.00	56.38	B	N
ATOM	11939	CD	PRO	766	76.833	34.541	62.831	1.00	56.67	B	C
ATOM	11940	CA	PRO	766	75.095	35.263	64.356	1.00	57.95	B	C
ATOM	11941	CB	PRO	766	74.509	34.544	63.141	1.00	58.24	B	C
ATOM	11942	CG	PRO	766	75.626	33.633	62.728	1.00	57.40	B	C
ATOM	11943	C	PRO	766	74.805	34.523	65.664	1.00	59.30	B	C
ATOM	11944	O	PRO	766	73.791	33.789	65.711	1.00	60.29	B	O
ATOM	11945	OXT	PRO	766	75.584	34.704	66.627	1.00	59.84	B	O
TER	11946		PRO	766						B	
ATOM	11947	C1	NAG	901	25.105	38.477	14.927	1.00	45.03	E	C
ATOM	11948	C2	NAG	901	26.266	38.501	13.922	1.00	45.16	E	C
ATOM	11949	N2	NAG	901	27.447	39.002	14.595	1.00	44.20	E	N
ATOM	11950	C7	NAG	901	28.662	38.702	14.153	1.00	43.63	E	C
ATOM	11951	O7	NAG	901	29.050	37.546	13.997	1.00	44.60	E	O
ATOM	11952	C8	NAG	901	29.588	39.864	13.838	1.00	43.83	E	C
ATOM	11953	C3	NAG	901	25.942	39.385	12.713	1.00	46.38	E	C
ATOM	11954	O3	NAG	901	26.953	39.235	11.728	1.00	49.49	E	O
ATOM	11955	C4	NAG	901	24.591	38.987	12.124	1.00	47.76	E	C

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(Continued)

## FIG. 4 - 245

ATOM	11956	04	NAG	901	24.256	39.836	11.036	1.00	49.01	E	0
ATOM	11957	C5	NAG	901	23.545	39.104	13.219	1.00	49.11	E	C
ATOM	11958	05	NAG	901	23.858	38.173	14.276	1.00	47.99	E	0
ATOM	11959	C6	NAG	901	22.143	38.804	12.731	1.00	50.99	E	C
ATOM	11960	06	NAG	901	21.706	39.781	11.793	1.00	53.28	E	0
ATOM	11961	C1	NAG	902	34.526	67.450	4.248	1.00	29.71	E	C
ATOM	11962	C2	NAG	902	33.682	66.990	3.051	1.00	31.02	E	C
ATOM	11963	N2	NAG	902	34.077	65.638	2.692	1.00	35.02	E	N
ATOM	11964	C7	NAG	902	33.181	64.660	2.610	1.00	35.78	E	C
ATOM	11965	07	NAG	902	32.213	64.701	1.852	1.00	37.59	E	0
ATOM	11966	C8	NAG	902	33.392	63.449	3.503	1.00	37.18	E	C
ATOM	11967	C3	NAG	902	33.927	67.915	1.848	1.00	31.67	E	C
ATOM	11968	03	NAG	902	33.032	67.583	0.794	1.00	34.76	E	0
ATOM	11969	C4	NAG	902	33.753	69.386	2.248	1.00	31.76	E	C
ATOM	11970	04	NAG	902	34.037	70.238	1.144	1.00	30.03	E	0
ATOM	11971	C5	NAG	902	34.701	69.674	3.412	1.00	30.64	E	C
ATOM	11972	05	NAG	902	34.332	68.844	4.526	1.00	30.02	E	0
ATOM	11973	C6	NAG	902	34.720	71.114	3.892	1.00	30.81	E	C
ATOM	11974	06	NAG	902	33.457	71.512	4.409	1.00	34.26	E	0
ATOM	11975	C1	NAG	903	64.239	77.734	14.341	1.00	27.20	E	C
ATOM	11976	C2	NAG	903	63.984	78.203	12.917	1.00	26.96	E	C
ATOM	11977	N2	NAG	903	63.551	77.080	12.116	1.00	25.19	E	N
ATOM	11978	C7	NAG	903	62.349	77.076	11.551	1.00	24.99	E	C
ATOM	11979	07	NAG	903	62.121	76.492	10.490	1.00	25.88	E	0
ATOM	11980	C8	NAG	903	61.222	77.800	12.272	1.00	23.55	E	C
ATOM	11981	C3	NAG	903	65.253	78.817	12.325	1.00	29.00	E	C
ATOM	11982	03	NAG	903	64.947	79.400	11.066	1.00	29.62	E	0
ATOM	11983	C4	NAG	903	65.814	79.900	13.248	1.00	30.83	E	C
ATOM	11984	04	NAG	903	67.092	80.316	12.778	1.00	31.15	E	0
ATOM	11985	C5	NAG	903	65.929	79.389	14.690	1.00	30.71	E	C
ATOM	11986	05	NAG	903	64.669	78.842	15.133	1.00	30.11	E	0
ATOM	11987	C6	NAG	903	66.276	80.502	15.659	1.00	32.26	E	C
ATOM	11988	06	NAG	903	65.937	80.144	16.993	1.00	35.52	E	0
ATOM	11989	C1	NAG	904	56.857	73.229	-0.933	1.00	21.65	E	C
ATOM	11990	C2	NAG	904	58.289	73.099	-1.475	1.00	21.59	E	C
ATOM	11991	N2	NAG	904	58.532	71.758	-1.961	1.00	21.40	E	N
ATOM	11992	C7	NAG	904	58.567	71.523	-3.267	1.00	20.76	E	C
ATOM	11993	07	NAG	904	58.745	72.412	-4.104	1.00	18.55	E	0
ATOM	11994	C8	NAG	904	58.371	70.080	-3.709	1.00	20.74	E	C
ATOM	11995	C3	NAG	904	59.325	73.441	-0.417	1.00	22.32	E	C
ATOM	11996	03	NAG	904	60.611	73.413	-1.009	1.00	22.81	E	0
ATOM	11997	C4	NAG	904	59.022	74.832	0.129	1.00	22.85	E	C
ATOM	11998	04	NAG	904	59.986	75.217	1.101	1.00	24.62	E	0
ATOM	11999	C5	NAG	904	57.634	74.781	0.737	1.00	22.86	E	C
ATOM	12000	05	NAG	904	56.672	74.506	-0.297	1.00	21.95	E	0
ATOM	12001	C6	NAG	904	57.232	76.083	1.385	1.00	24.39	E	C
ATOM	12002	06	NAG	904	57.196	77.133	0.430	1.00	31.81	E	0
ATOM	12003	C1	NAG	905	49.743	85.075	37.084	1.00	31.93	E	C
ATOM	12004	C2	NAG	905	49.010	86.230	37.756	1.00	33.35	E	C

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(Continued)

## FIG. 4 - 246

ATOM	12005	N2	NAG	905	47.823	86.586	37.012	1.00	34.30	E	N
ATOM	12006	C7	NAG	905	46.648	86.099	37.395	1.00	35.18	E	C
ATOM	12007	07	NAG	905	46.362	85.888	38.578	1.00	36.47	E	O
ATOM	12008	C8	NAG	905	45.640	85.786	36.303	1.00	37.15	E	C
ATOM	12009	C3	NAG	905	49.951	87.416	37.924	1.00	33.45	E	C
ATOM	12010	03	NAG	905	49.256	88.512	38.495	1.00	33.93	E	O
ATOM	12011	C4	NAG	905	51.043	86.945	38.863	1.00	35.37	E	C
ATOM	12012	04	NAG	905	51.934	88.009	39.193	1.00	35.45	E	O
ATOM	12013	C5	NAG	905	51.794	85.773	38.215	1.00	34.39	E	C
ATOM	12014	05	NAG	905	50.878	84.684	37.887	1.00	32.56	E	O
ATOM	12015	C6	NAG	905	52.787	85.212	39.214	1.00	36.29	E	C
ATOM	12016	06	NAG	905	52.150	84.936	40.459	1.00	35.52	E	O
ATOM	12017	C1	NAG	906	128.439	74.792	56.371	1.00	36.45	E	C
ATOM	12018	C2	NAG	906	127.977	75.856	55.375	1.00	37.00	E	C
ATOM	12019	N2	NAG	906	126.880	75.335	54.586	1.00	37.17	E	N
ATOM	12020	C7	NAG	906	125.666	75.871	54.690	1.00	38.41	E	C
ATOM	12021	07	NAG	906	125.264	76.427	55.714	1.00	38.52	E	O
ATOM	12022	C8	NAG	906	124.760	75.782	53.471	1.00	36.25	E	C
ATOM	12023	C3	NAG	906	129.133	76.265	54.465	1.00	38.66	E	C
ATOM	12024	03	NAG	906	128.723	77.334	53.625	1.00	39.59	E	O
ATOM	12025	C4	NAG	906	130.331	76.704	55.308	1.00	39.58	E	C
ATOM	12026	04	NAG	906	131.439	76.975	54.460	1.00	41.48	E	O
ATOM	12027	C5	NAG	906	130.699	75.602	56.312	1.00	40.24	E	C
ATOM	12028	05	NAG	906	129.556	75.268	57.133	1.00	38.27	E	O
ATOM	12029	C6	NAG	906	131.811	76.032	57.255	1.00	41.89	E	C
ATOM	12030	06	NAG	906	131.906	75.162	58.378	1.00	46.70	E	O
ATOM	12031	C1	NAG	907	126.770	72.294	25.405	1.00	33.54	E	C
ATOM	12032	C2	NAG	907	127.763	73.454	25.478	1.00	35.73	E	C
ATOM	12033	N2	NAG	907	127.401	74.367	26.540	1.00	37.97	E	N
ATOM	12034	C7	NAG	907	128.139	74.400	27.644	1.00	41.34	E	C
ATOM	12035	07	NAG	907	128.715	73.403	28.094	1.00	42.96	E	O
ATOM	12036	C8	NAG	907	128.278	75.739	28.352	1.00	42.60	E	C
ATOM	12037	C3	NAG	907	127.776	74.167	24.126	1.00	36.63	E	C
ATOM	12038	03	NAG	907	128.692	75.253	24.154	1.00	38.28	E	O
ATOM	12039	C4	NAG	907	128.171	73.148	23.047	1.00	35.89	E	C
ATOM	12040	04	NAG	907	128.191	73.758	21.763	1.00	35.82	E	O
ATOM	12041	C5	NAG	907	127.161	71.995	23.075	1.00	35.12	E	C
ATOM	12042	05	NAG	907	127.166	71.377	24.380	1.00	32.61	E	O
ATOM	12043	C6	NAG	907	127.444	70.913	22.057	1.00	36.17	E	C
ATOM	12044	06	NAG	907	128.515	70.083	22.478	1.00	38.44	E	O
ATOM	12045	C1	NAG	908	97.567	64.129	12.586	1.00	33.83	E	C
ATOM	12046	C2	NAG	908	98.226	65.101	11.602	1.00	36.51	E	C
ATOM	12047	N2	NAG	908	98.466	66.365	12.269	1.00	40.33	E	N
ATOM	12048	C7	NAG	908	99.645	66.962	12.148	1.00	43.03	E	C
ATOM	12049	07	NAG	908	100.703	66.434	12.500	1.00	45.77	E	O
ATOM	12050	C8	NAG	908	99.655	68.349	11.529	1.00	43.86	E	C
ATOM	12051	C3	NAG	908	97.328	65.325	10.380	1.00	37.11	E	C
ATOM	12052	03	NAG	908	98.013	66.122	9.426	1.00	37.35	E	O
ATOM	12053	C4	NAG	908	96.945	63.975	9.760	1.00	36.97	E	C

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(Continued)

## FIG. 4 - 247

ATOM	12054	04	NAG	908	96.049	64.165	8.668	1.00	36.08	E	0
ATOM	12055	C5	NAG	908	96.291	63.106	10.841	1.00	35.43	E	C
ATOM	12056	05	NAG	908	97.215	62.906	11.930	1.00	33.34	E	0
ATOM	12057	C6	NAG	908	95.890	61.735	10.341	1.00	36.72	E	C
ATOM	12058	06	NAG	908	95.085	61.057	11.296	1.00	38.75	E	0
ATOM	12059	C1	NAG	909	106.501	80.407	11.987	1.00	55.21	E	C
ATOM	12060	C2	NAG	909	105.627	81.255	11.048	1.00	55.75	E	C
ATOM	12061	N2	NAG	909	105.631	82.658	11.427	1.00	55.80	E	N
ATOM	12062	C7	NAG	909	106.748	83.259	11.828	1.00	56.83	E	C
ATOM	12063	07	NAG	909	107.685	83.526	11.066	1.00	55.16	E	0
ATOM	12064	C8	NAG	909	106.838	83.620	13.305	1.00	56.25	E	C
ATOM	12065	C3	NAG	909	104.195	80.724	11.087	1.00	56.36	E	C
ATOM	12066	03	NAG	909	103.396	81.452	10.166	1.00	58.58	E	0
ATOM	12067	C4	NAG	909	104.176	79.229	10.744	1.00	56.19	E	C
ATOM	12068	04	NAG	909	102.855	78.716	10.862	1.00	55.29	E	0
ATOM	12069	C5	NAG	909	105.117	78.478	11.692	1.00	56.24	E	C
ATOM	12070	05	NAG	909	106.446	79.028	11.600	1.00	56.65	E	0
ATOM	12071	C6	NAG	909	105.230	76.996	11.381	1.00	57.38	E	C
ATOM	12072	06	NAG	909	106.370	76.423	12.010	1.00	55.01	E	0
ATOM	12073	C1	NAG	910	105.213	38.428	20.006	1.00	34.33	E	C
ATOM	12074	C2	NAG	910	106.113	37.293	19.498	1.00	37.27	E	C
ATOM	12075	N2	NAG	910	107.447	37.789	19.211	1.00	40.05	E	N
ATOM	12076	C7	NAG	910	108.495	36.984	19.368	1.00	42.24	E	C
ATOM	12077	07	NAG	910	109.013	36.771	20.465	1.00	42.65	E	0
ATOM	12078	C8	NAG	910	109.047	36.295	18.126	1.00	42.65	E	C
ATOM	12079	C3	NAG	910	105.504	36.650	18.245	1.00	37.60	E	C
ATOM	12080	03	NAG	910	106.296	35.547	17.831	1.00	38.44	E	0
ATOM	12081	C4	NAG	910	104.084	36.182	18.551	1.00	36.63	E	C
ATOM	12082	04	NAG	910	103.489	35.616	17.388	1.00	37.52	E	0
ATOM	12083	C5	NAG	910	103.274	37.387	19.037	1.00	35.81	E	C
ATOM	12084	05	NAG	910	103.883	37.930	20.229	1.00	34.96	E	0
ATOM	12085	C6	NAG	910	101.838	37.042	19.385	1.00	34.79	E	C
ATOM	12086	06	NAG	910	101.781	36.089	20.437	1.00	34.77	E	0
TER	12087		NAG	910						E	
ATOM	12088	0	HOH	1	53.435	80.704	18.172	1.00	10.60	W	0
ATOM	12089	0	HOH	2	57.473	78.703	26.320	1.00	21.03	W	0
ATOM	12090	0	HOH	3	65.386	56.077	37.040	1.00	7.09	W	0
ATOM	12091	0	HOH	4	56.235	76.520	22.816	1.00	14.76	W	0
ATOM	12092	0	HOH	5	58.127	60.758	28.066	1.00	4.57	W	0
ATOM	12093	0	HOH	6	40.099	59.877	48.410	1.00	16.00	W	0
ATOM	12094	0	HOH	7	29.796	47.323	37.410	1.00	24.76	W	0
ATOM	12095	0	HOH	8	38.634	67.195	51.371	1.00	22.65	W	0
ATOM	12096	0	HOH	9	41.732	52.103	37.673	1.00	13.34	W	0
ATOM	12097	0	HOH	10	79.275	54.159	21.409	1.00	15.53	W	0
ATOM	12098	0	HOH	11	65.287	66.160	35.128	1.00	7.29	W	0
ATOM	12099	0	HOH	12	79.267	49.364	26.780	1.00	14.00	W	0
ATOM	12100	0	HOH	13	67.989	56.792	26.833	1.00	20.21	W	0
ATOM	12101	0	HOH	14	68.995	70.138	19.815	1.00	12.98	W	0
ATOM	12102	0	HOH	15	59.193	63.441	21.787	1.00	5.68	W	0

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(Continued)

## FIG. 4 - 248

ATOM	12103	0	HOH	16	49.896	66.700	47.886	1.00	13.21	W	0
ATOM	12104	0	HOH	17	48.544	53.043	50.567	1.00	20.65	W	0
ATOM	12105	0	HOH	18	73.938	69.817	52.424	1.00	34.74	W	0
ATOM	12106	0	HOH	19	36.883	69.650	29.378	1.00	25.18	W	0
ATOM	12107	0	HOH	20	50.912	61.115	48.431	1.00	18.77	W	0
ATOM	12108	0	HOH	21	58.369	85.282	28.107	1.00	27.06	W	0
ATOM	12109	0	HOH	22	62.886	63.930	21.686	1.00	29.16	W	0
ATOM	12110	0	HOH	23	43.777	87.394	23.730	1.00	9.96	W	0
ATOM	12111	0	HOH	24	48.078	67.109	30.405	1.00	21.66	W	0
ATOM	12112	0	HOH	25	36.753	80.303	31.025	1.00	34.33	W	0
ATOM	12113	0	HOH	26	63.225	66.634	22.568	1.00	10.18	W	0
ATOM	12114	0	HOH	27	35.078	54.838	52.427	1.00	29.90	W	0
ATOM	12115	0	HOH	28	57.184	80.961	23.145	1.00	17.51	W	0
ATOM	12116	0	HOH	29	73.677	71.484	27.824	1.00	34.92	W	0
ATOM	12117	0	HOH	30	76.251	57.060	34.794	1.00	28.05	W	0
ATOM	12118	0	HOH	31	72.985	72.092	24.987	1.00	14.46	W	0
ATOM	12119	0	HOH	32	61.839	84.543	25.502	1.00	22.75	W	0
ATOM	12120	0	HOH	33	33.787	63.840	46.551	1.00	12.55	W	0
ATOM	12121	0	HOH	34	47.827	47.441	47.587	1.00	25.33	W	0
ATOM	12122	0	HOH	35	55.562	56.510	44.904	1.00	30.51	W	0
ATOM	12123	0	HOH	36	31.114	59.222	42.224	1.00	13.22	W	0
ATOM	12124	0	HOH	37	82.143	64.199	47.510	1.00	21.69	W	0
ATOM	12125	0	HOH	38	41.587	70.385	33.904	1.00	24.19	W	0
ATOM	12126	0	HOH	39	70.447	47.056	34.998	1.00	24.19	W	0
ATOM	12127	0	HOH	40	23.146	49.571	32.910	1.00	22.85	W	0
ATOM	12128	0	HOH	41	23.427	53.516	39.573	1.00	12.47	W	0
ATOM	12129	0	HOH	42	74.977	48.248	21.021	1.00	24.35	W	0
ATOM	12130	0	HOH	43	81.171	53.457	19.457	1.00	32.23	W	0
ATOM	12131	0	HOH	44	70.982	61.003	21.232	1.00	19.07	W	0
ATOM	12132	0	HOH	45	51.713	50.325	19.619	1.00	36.05	W	0
ATOM	12133	0	HOH	46	75.424	58.001	59.062	1.00	20.53	W	0
ATOM	12134	0	HOH	47	52.251	54.978	15.598	1.00	20.74	W	0
ATOM	12135	0	HOH	48	37.551	51.103	23.882	1.00	16.65	W	0
ATOM	12136	0	HOH	49	31.428	66.281	21.097	1.00	18.82	W	0
ATOM	12137	0	HOH	50	45.546	72.589	-9.525	1.00	19.51	W	0
ATOM	12138	0	HOH	51	71.765	47.337	39.374	1.00	16.49	W	0
ATOM	12139	0	HOH	52	57.328	68.673	61.331	1.00	26.41	W	0
ATOM	12140	0	HOH	53	72.778	48.947	47.621	1.00	17.49	W	0
ATOM	12141	0	HOH	54	30.292	82.021	10.956	1.00	24.56	W	0
ATOM	12142	0	HOH	55	47.165	45.427	40.043	1.00	35.52	W	0
ATOM	12143	0	HOH	56	25.673	60.491	43.209	1.00	10.79	W	0
ATOM	12144	0	HOH	57	71.617	62.843	34.752	1.00	17.19	W	0
ATOM	12145	0	HOH	58	46.059	55.643	2.123	1.00	19.51	W	0
ATOM	12146	0	HOH	59	68.766	45.985	50.017	1.00	22.18	W	0
ATOM	12147	0	HOH	60	52.732	70.566	0.317	1.00	32.17	W	0
ATOM	12148	0	HOH	61	61.782	69.597	25.094	1.00	13.27	W	0
ATOM	12149	0	HOH	62	51.352	79.521	14.538	1.00	17.25	W	0
ATOM	12150	0	HOH	63	48.267	86.907	16.122	1.00	21.54	W	0
ATOM	12151	0	HOH	64	49.536	54.337	14.938	1.00	22.27	W	0

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## FIG. 4 - 249

(Continued)

ATOM	12152	0	HOH	65	37.711	84.458	31.782	1.00	38.65	W	0
ATOM	12153	0	HOH	66	41.832	62.441	48.190	1.00	23.50	W	0
ATOM	12154	0	HOH	67	56.514	63.214	39.402	1.00	20.39	W	0
ATOM	12155	0	HOH	68	48.166	60.456	42.122	1.00	37.55	W	0
ATOM	12156	0	HOH	69	52.076	51.584	45.757	1.00	22.02	W	0
ATOM	12157	0	HOH	70	47.607	61.634	15.612	1.00	34.50	W	0
ATOM	12158	0	HOH	71	39.108	76.636	34.882	1.00	24.21	W	0
ATOM	12159	0	HOH	72	62.894	85.163	44.724	1.00	38.05	W	0
ATOM	12160	0	HOH	73	49.937	51.963	48.658	1.00	25.50	W	0
ATOM	12161	0	HOH	74	32.972	63.405	9.645	1.00	31.16	W	0
ATOM	12162	0	HOH	75	76.481	50.940	55.523	1.00	8.02	W	0
ATOM	12163	0	HOH	76	54.751	68.666	-3.038	1.00	19.33	W	0
ATOM	12164	0	HOH	77	69.797	76.851	37.550	1.00	38.44	W	0
ATOM	12165	0	HOH	78	60.195	69.793	56.043	1.00	27.75	W	0
ATOM	12166	0	HOH	79	68.721	77.775	28.423	1.00	14.61	W	0
ATOM	12167	0	HOH	80	76.538	41.044	29.727	1.00	24.17	W	0
ATOM	12168	0	HOH	81	27.643	63.804	39.245	1.00	20.70	W	0
ATOM	12169	0	HOH	82	42.573	57.621	42.066	1.00	19.56	W	0
ATOM	12170	0	HOH	83	51.219	56.139	24.829	1.00	41.31	W	0
ATOM	12171	0	HOH	84	64.281	54.295	25.797	1.00	15.83	W	0
ATOM	12172	0	HOH	85	48.093	54.052	46.307	1.00	38.41	W	0
ATOM	12173	0	HOH	86	37.006	52.225	21.202	1.00	23.83	W	0
ATOM	12174	0	HOH	87	44.149	74.948	5.314	1.00	17.55	W	0
ATOM	12175	0	HOH	88	72.912	75.091	28.633	1.00	25.98	W	0
ATOM	12176	0	HOH	89	52.329	67.860	33.481	1.00	8.31	W	0
ATOM	12177	0	HOH	90	66.266	74.773	42.238	1.00	16.00	W	0
ATOM	12178	0	HOH	91	59.283	77.076	9.072	1.00	41.29	W	0
ATOM	12179	0	HOH	92	77.526	46.454	20.254	1.00	34.51	W	0
ATOM	12180	0	HOH	93	59.751	56.673	29.191	1.00	24.40	W	0
ATOM	12181	0	HOH	94	43.531	63.248	14.122	1.00	22.64	W	0
ATOM	12182	0	HOH	95	56.677	73.257	-8.550	1.00	18.65	W	0
ATOM	12183	0	HOH	96	64.366	82.016	33.202	1.00	24.81	W	0
ATOM	12184	0	HOH	97	58.839	62.776	26.537	1.00	11.00	W	0
ATOM	12185	0	HOH	98	52.478	72.152	3.092	1.00	13.58	W	0
ATOM	12186	0	HOH	99	59.860	59.389	29.429	1.00	20.06	W	0
ATOM	12187	0	HOH	100	64.047	73.184	44.557	1.00	15.66	W	0
ATOM	12188	0	HOH	101	44.369	74.978	38.087	1.00	11.11	W	0
ATOM	12189	0	HOH	102	61.861	50.833	14.510	1.00	31.09	W	0
ATOM	12190	0	HOH	103	40.708	73.940	22.137	1.00	13.81	W	0
ATOM	12191	0	HOH	104	51.853	81.601	16.339	1.00	16.73	W	0
ATOM	12192	0	HOH	105	59.699	55.348	63.144	1.00	20.67	W	0
ATOM	12193	0	HOH	106	45.186	81.560	8.416	1.00	13.89	W	0
ATOM	12194	0	HOH	107	37.516	59.183	48.946	1.00	20.72	W	0
ATOM	12195	0	HOH	108	22.032	56.444	27.934	1.00	30.26	W	0
ATOM	12196	0	HOH	109	65.773	63.945	59.504	1.00	15.82	W	0
ATOM	12197	0	HOH	110	45.931	73.798	1.832	1.00	25.56	W	0
ATOM	12198	0	HOH	111	29.602	40.898	24.033	1.00	25.93	W	0
ATOM	12199	0	HOH	112	19.080	57.313	26.663	1.00	20.07	W	0
ATOM	12200	0	HOH	113	61.355	50.296	11.653	1.00	20.49	W	0

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(Continued)

## FIG. 4 - 250

ATOM	12201	0	HOH	114	41.491	58.601	0.047	1.00	42.91	W	0
ATOM	12202	0	HOH	115	64.362	64.567	16.259	1.00	24.97	W	0
ATOM	12203	0	HOH	116	43.928	76.242	2.332	1.00	21.69	W	0
ATOM	12204	0	HOH	117	80.703	69.349	43.827	1.00	28.64	W	0
ATOM	12205	0	HOH	118	81.671	48.368	20.456	1.00	15.16	W	0
ATOM	12206	0	HOH	119	59.413	71.127	54.004	1.00	22.01	W	0
ATOM	12207	0	HOH	120	27.474	69.426	47.288	1.00	26.74	W	0
ATOM	12208	0	HOH	121	69.871	60.279	33.380	1.00	13.47	W	0
ATOM	12209	0	HOH	122	67.879	38.425	47.297	1.00	25.68	W	0
ATOM	12210	0	HOH	123	41.866	62.152	36.306	1.00	27.91	W	0
ATOM	12211	0	HOH	124	82.055	50.923	20.718	1.00	23.09	W	0
ATOM	12212	0	HOH	125	38.821	82.651	33.998	1.00	14.04	W	0
ATOM	12213	0	HOH	126	64.420	42.195	31.710	1.00	28.88	W	0
ATOM	12214	0	HOH	127	60.713	36.262	43.885	1.00	22.95	W	0
ATOM	12215	0	HOH	128	63.095	38.041	44.744	1.00	26.42	W	0
ATOM	12216	0	HOH	129	36.718	65.633	50.633	1.00	38.12	W	0
ATOM	12217	0	HOH	130	55.575	80.086	20.196	1.00	26.23	W	0
ATOM	12218	0	HOH	131	41.981	65.129	15.577	1.00	23.62	W	0
ATOM	12219	0	HOH	132	48.067	75.632	53.563	1.00	36.38	W	0
ATOM	12220	0	HOH	133	75.617	59.792	32.116	1.00	35.58	W	0
ATOM	12221	0	HOH	134	73.522	67.486	30.484	1.00	21.07	W	0
ATOM	12222	0	HOH	135	65.965	81.671	30.091	1.00	41.74	W	0
ATOM	12223	0	HOH	136	41.663	53.300	13.574	1.00	39.95	W	0
ATOM	12224	0	HOH	137	42.885	39.029	29.960	1.00	29.57	W	0
ATOM	12225	0	HOH	138	67.606	56.683	24.253	1.00	37.19	W	0
ATOM	12226	0	HOH	139	138.150	54.591	37.133	1.00	19.60	W	0
ATOM	12227	0	HOH	140	76.640	48.505	51.547	1.00	22.87	W	0
ATOM	12228	0	HOH	141	105.346	35.319	45.478	1.00	6.28	W	0
ATOM	12229	0	HOH	142	108.946	33.058	43.850	1.00	17.18	W	0
ATOM	12230	0	HOH	143	101.384	50.291	32.321	1.00	12.25	W	0
ATOM	12231	0	HOH	144	83.691	56.732	33.886	1.00	18.52	W	0
ATOM	12232	0	HOH	145	96.721	59.108	34.335	1.00	14.59	W	0
ATOM	12233	0	HOH	146	122.411	66.436	57.099	1.00	19.53	W	0
ATOM	12234	0	HOH	147	107.303	38.674	48.678	1.00	12.12	W	0
ATOM	12235	0	HOH	148	102.207	54.174	15.770	1.00	18.02	W	0
ATOM	12236	0	HOH	149	104.534	49.338	27.730	1.00	13.93	W	0
ATOM	12237	0	HOH	150	113.995	67.497	30.740	1.00	26.00	W	0
ATOM	12238	0	HOH	151	115.903	54.147	45.005	1.00	10.46	W	0
ATOM	12239	0	HOH	152	114.104	55.650	9.401	1.00	27.03	W	0
ATOM	12240	0	HOH	153	86.360	55.414	40.305	1.00	14.32	W	0
ATOM	12241	0	HOH	154	97.554	40.670	45.200	1.00	18.35	W	0
ATOM	12242	0	HOH	155	119.087	37.761	27.531	1.00	31.02	W	0
ATOM	12243	0	HOH	156	87.809	62.914	36.962	1.00	26.29	W	0
ATOM	12244	0	HOH	157	83.356	65.229	44.012	1.00	37.02	W	0
ATOM	12245	0	HOH	158	98.650	46.435	54.377	1.00	26.11	W	0
ATOM	12246	0	HOH	159	99.982	40.104	43.504	1.00	11.71	W	0
ATOM	12247	0	HOH	160	122.550	42.243	44.636	1.00	14.84	W	0
ATOM	12248	0	HOH	161	101.404	56.669	35.498	1.00	35.54	W	0
ATOM	12249	0	HOH	162	88.481	51.896	31.163	1.00	12.64	W	0

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## FIG. 4 - 251

(Continued)

ATOM	12250	0	HOH	163	95.169	58.602	25.005	1.00	10.78	W	0
ATOM	12251	0	HOH	164	115.235	34.630	45.444	1.00	26.24	W	0
ATOM	12252	0	HOH	165	106.826	53.003	55.571	1.00	20.62	W	0
ATOM	12253	0	HOH	166	84.875	59.299	19.482	1.00	36.24	W	0
ATOM	12254	0	HOH	167	113.139	50.670	46.942	1.00	20.56	W	0
ATOM	12255	0	HOH	168	95.042	48.091	37.270	1.00	21.34	W	0
ATOM	12256	0	HOH	169	76.879	72.537	31.569	1.00	23.37	W	0
ATOM	12257	0	HOH	170	114.148	58.106	48.086	1.00	18.43	W	0
ATOM	12258	0	HOH	171	89.134	33.853	32.584	1.00	22.93	W	0
ATOM	12259	0	HOH	172	104.484	32.367	28.628	1.00	23.01	W	0
ATOM	12260	0	HOH	173	97.990	56.523	56.950	1.00	35.07	W	0
ATOM	12261	0	HOH	174	108.093	59.050	11.178	1.00	23.37	W	0
ATOM	12262	0	HOH	175	95.968	47.759	51.786	1.00	19.27	W	0
ATOM	12263	0	HOH	176	93.653	58.234	55.683	1.00	19.54	W	0
ATOM	12264	0	HOH	177	117.454	64.613	44.832	1.00	25.55	W	0
ATOM	12265	0	HOH	178	96.322	67.790	27.707	1.00	29.36	W	0
ATOM	12266	0	HOH	179	80.831	40.760	23.388	1.00	28.01	W	0
ATOM	12267	0	HOH	180	109.521	38.188	50.278	1.00	16.30	W	0
ATOM	12268	0	HOH	181	88.081	40.289	29.465	1.00	7.47	W	0
ATOM	12269	0	HOH	182	112.135	42.102	29.409	1.00	28.14	W	0
ATOM	12270	0	HOH	183	110.546	33.279	45.877	1.00	22.55	W	0
ATOM	12271	0	HOH	184	101.361	45.858	44.078	1.00	28.83	W	0
ATOM	12272	0	HOH	185	126.633	38.023	29.778	1.00	31.97	W	0
ATOM	12273	0	HOH	186	122.283	37.257	34.566	1.00	18.77	W	0
ATOM	12274	0	HOH	187	99.753	38.623	40.032	1.00	18.28	W	0
ATOM	12275	0	HOH	188	122.547	56.954	36.341	1.00	20.05	W	0
ATOM	12276	0	HOH	189	68.079	78.219	33.025	1.00	38.49	W	0
ATOM	12277	0	HOH	190	134.519	46.667	45.989	1.00	34.45	W	0
ATOM	12278	0	HOH	191	110.945	39.354	35.865	1.00	10.27	W	0
ATOM	12279	0	HOH	192	118.982	51.843	57.881	1.00	13.62	W	0
ATOM	12280	0	HOH	193	123.824	35.631	32.830	1.00	19.19	W	0
ATOM	12281	0	HOH	194	100.524	45.123	38.393	1.00	26.68	W	0
ATOM	12282	0	HOH	195	122.815	60.696	63.937	1.00	24.15	W	0
ATOM	12283	0	HOH	196	96.208	59.856	31.652	1.00	12.71	W	0
ATOM	12284	0	HOH	197	80.023	56.246	54.587	1.00	10.61	W	0
ATOM	12285	0	HOH	198	109.915	41.219	37.675	1.00	19.28	W	0
ATOM	12286	0	HOH	199	96.990	75.649	27.926	1.00	9.03	W	0
ATOM	12287	0	HOH	200	103.494	44.373	34.046	1.00	8.20	W	0
ATOM	12288	0	HOH	201	97.045	44.873	53.124	1.00	15.97	W	0
ATOM	12289	0	HOH	202	109.135	58.341	13.499	1.00	22.83	W	0
ATOM	12290	0	HOH	203	96.465	39.089	47.689	1.00	12.68	W	0
ATOM	12291	0	HOH	204	99.669	54.200	16.885	1.00	13.83	W	0
ATOM	12292	0	HOH	205	85.350	34.351	33.261	1.00	15.83	W	0
ATOM	12293	0	HOH	206	106.252	38.178	46.273	1.00	17.78	W	0
ATOM	12294	0	HOH	207	102.838	63.592	15.944	1.00	23.96	W	0
ATOM	12295	0	HOH	208	114.173	52.027	44.587	1.00	12.16	W	0
ATOM	12296	0	HOH	209	114.209	49.450	36.803	1.00	19.70	W	0
ATOM	12297	0	HOH	210	78.079	55.141	59.990	1.00	33.63	W	0
ATOM	12298	0	HOH	211	95.004	41.032	14.678	1.00	29.66	W	0

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(Continued)

## FIG. 4-252

ATOM	12299	0	HOH	212	113.170	36.816	43.347	1.00	21.90	W	0
ATOM	12300	0	HOH	213	77.770	71.277	45.572	1.00	31.73	W	0
ATOM	12301	0	HOH	214	128.636	66.746	61.783	1.00	37.87	W	0
ATOM	12302	0	HOH	215	128.566	42.261	18.644	1.00	26.65	W	0
ATOM	12303	0	HOH	216	135.349	43.830	34.280	1.00	24.69	W	0
ATOM	12304	0	HOH	217	85.640	67.686	27.706	1.00	32.33	W	0
ATOM	12305	0	HOH	218	93.669	46.427	45.506	1.00	24.39	W	0
ATOM	12306	0	HOH	219	117.990	67.819	59.317	1.00	20.28	W	0
ATOM	12307	0	HOH	220	79.954	55.009	62.309	1.00	19.13	W	0
ATOM	12308	0	HOH	221	117.228	62.083	29.483	1.00	29.50	W	0
ATOM	12309	0	HOH	222	105.505	51.938	31.912	1.00	35.19	W	0
ATOM	12310	0	HOH	223	106.835	57.215	14.677	1.00	21.77	W	0
ATOM	12311	0	HOH	224	107.489	60.380	64.395	1.00	24.53	W	0
ATOM	12312	0	HOH	225	79.753	74.355	37.799	1.00	35.35	W	0
ATOM	12313	0	HOH	226	116.807	64.679	29.466	1.00	24.83	W	0
ATOM	12314	0	HOH	227	87.239	52.355	64.706	1.00	21.19	W	0
ATOM	12315	0	HOH	228	81.916	67.988	41.878	1.00	14.54	W	0
ATOM	12316	0	HOH	229	106.295	62.226	36.826	1.00	26.06	W	0
ATOM	12317	0	HOH	230	78.057	49.553	53.991	1.00	15.40	W	0
ATOM	12318	0	HOH	231	99.797	47.673	22.572	1.00	18.00	W	0
ATOM	12319	0	HOH	232	80.925	62.495	37.326	1.00	9.28	W	0
ATOM	12320	0	HOH	233	93.378	45.857	52.934	1.00	12.13	W	0
ATOM	12321	0	HOH	234	132.069	46.877	33.339	1.00	20.97	W	0
ATOM	12322	0	HOH	235	93.916	62.211	25.521	1.00	13.10	W	0
ATOM	12323	0	HOH	236	93.249	60.882	37.895	1.00	26.19	W	0
ATOM	12324	0	HOH	237	100.380	52.169	18.636	1.00	7.98	W	0
ATOM	12325	0	HOH	238	82.096	55.169	32.059	1.00	10.45	W	0
ATOM	12326	0	HOH	239	94.471	48.635	53.699	1.00	13.21	W	0
ATOM	12327	0	HOH	240	87.009	55.227	64.894	1.00	24.88	W	0
ATOM	12328	0	HOH	241	95.857	52.760	15.499	1.00	29.83	W	0
ATOM	12329	0	HOH	242	117.688	49.829	33.274	1.00	13.15	W	0
ATOM	12330	0	HOH	243	103.675	56.528	15.602	1.00	19.17	W	0
ATOM	12331	0	HOH	244	99.571	37.563	42.732	1.00	22.69	W	0
ATOM	12332	0	HOH	245	100.413	48.087	60.147	1.00	23.84	W	0
ATOM	12333	0	HOH	246	117.307	73.448	16.262	1.00	29.45	W	0
ATOM	12334	0	HOH	247	124.287	57.265	34.284	1.00	15.90	W	0
ATOM	12335	0	HOH	248	124.770	56.884	15.714	1.00	26.61	W	0
ATOM	12336	0	HOH	249	133.182	57.356	30.667	1.00	8.25	W	0
ATOM	12337	0	HOH	250	106.948	46.114	47.228	1.00	18.40	W	0
ATOM	12338	0	HOH	251	101.409	54.086	55.370	1.00	24.76	W	0
ATOM	12339	0	HOH	252	116.022	62.795	46.555	1.00	17.19	W	0
ATOM	12340	0	HOH	253	95.637	65.687	28.739	1.00	22.07	W	0
ATOM	12341	0	HOH	254	89.440	32.347	36.665	1.00	21.89	W	0
ATOM	12342	0	HOH	255	86.628	29.295	53.611	1.00	28.08	W	0
ATOM	12343	0	HOH	256	102.111	48.926	69.771	1.00	28.02	W	0
ATOM	12344	0	HOH	257	117.835	65.790	61.089	1.00	30.23	W	0
ATOM	12345	0	HOH	258	105.286	61.859	63.757	1.00	33.92	W	0
ATOM	12346	0	HOH	259	86.743	64.218	34.930	1.00	28.91	W	0
ATOM	12347	0	HOH	260	105.249	47.160	40.635	1.00	20.28	W	0

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## F I G. 4 - 2 5 3

(Continued)

ATOM	12348	0	HOH	261	125.748	77.301	50.793	1.00	32.51	W	0
ATOM	12349	0	HOH	262	73.839	74.279	32.315	1.00	30.75	W	0
ATOM	12350	0	HOH	263	92.355	54.248	49.336	1.00	32.87	W	0
ATOM	12351	0	HOH	264	102.237	61.200	14.237	1.00	31.77	W	0
ATOM	12352	0	HOH	265	111.596	65.302	59.180	1.00	14.35	W	0
ATOM	12353	0	HOH	266	76.203	36.588	32.586	1.00	25.41	W	0
ATOM	12354	0	HOH	267	95.406	54.983	52.304	1.00	31.62	W	0
ATOM	12355	0	HOH	268	71.413	36.734	46.233	1.00	28.42	W	0
ATOM	12356	0	HOH	269	127.938	49.749	55.356	1.00	31.01	W	0
ATOM	12357	0	HOH	270	122.216	58.021	31.710	1.00	35.14	W	0
ATOM	12358	0	HOH	271	94.659	59.753	40.284	1.00	27.37	W	0
ATOM	12359	0	HOH	272	77.118	34.975	51.599	1.00	37.45	W	0
ATOM	12360	0	HOH	273	112.752	32.790	41.771	1.00	30.32	W	0
TER	12361		HOH	273						W	
END											

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## SEQUENCE LISTING

<110> TANABE SEIYAKU CO., LTD.

<120> Three-dimensional structure of dipeptidyl peptidase IV

<130> 03-039-PCT

<150> US 60/398,761

<151> 2002-07-29

<160> 2

<170> PatentIn version 3.1

<210> 1

<211> 2301

<212> DNA

<213> Homo sapiens

<220>

<221> CDS

<222> (1)..(2301)

<223>

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48

2/11

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 1 5 10 15  
 ctt gtc acc atc atc acc gtg ccc gtg gtt ctg ctg aac aaa ggc aca 96  
 Leu Val Thr Ile Ile Thr Val Pro Val Val Leu Leu Asn Lys Gly Thr  
 20 25 30  
 gat gat gct aca gct gac agt cgc aaa act tac act cta act gat tac 144  
 Asp Asp Ala Thr Ala Asp Ser Arg Lys Thr Tyr Thr Leu Thr Asp Tyr  
 35 40 45  
 tta aaa aat act tat aga ctg aag tta tac tcc tta aga tgg att tca 192  
 Leu Lys Asn Thr Tyr Arg Leu Lys Leu Tyr Ser Leu Arg Trp Ile Ser  
 50 55 60  
 gat cat gaa tat ctc tac aaa caa gaa aat aat atc ttg gta ttc aat 240  
 Asp His Glu Tyr Leu Tyr Lys Gln Glu Asn Asn Ile Leu Val Phe Asn  
 65 70 75 80  
 gct gaa tat gga aac agc tca gtt ttc ttg gag aac agt aca ttt gat 288  
 Ala Glu Tyr Gly Asn Ser Ser Val Phe Leu Glu Asn Ser Thr Phe Asp  
 85 90 95  
 gag ttt gga cat tct atc aat gat tat tca ata tct cct gat ggg cag 336  
 Glu Phe Gly His Ser Ile Asn Asp Tyr Ser Ile Ser Pro Asp Gly Gln  
 100 105 110  
 ttt att ctc tta gaa tac aac tac gtg aag caa tgg agg cat tcc tac 384  
 Phe Ile Leu Leu Glu Tyr Asn Tyr Val Lys Gln Trp Arg His Ser Tyr  
 115 120 125  
 aca gct tca tat gac att tat gat tta aat aaa agg cag ctg att aca 432  
 Thr Ala Ser Tyr Asp Ile Tyr Asp Leu Asn Lys Arg Gln Leu Ile Thr  
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 gaa gag agg att cca aac aac aca cag tgg gtc aca tgg tca cca gtg 480

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[illegible]

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Ala Pro Ala Ser Met Leu Ile Gly Asp His Tyr Leu Cys Asp Val Thr	
290	295
300	
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Trp Ala Thr Gln Glu Arg Ile Ser Leu Gln Trp Leu Arg Arg Ile Gln	
305	310
315	320
aac tat tgc gtc atg gat att tgt gac tat gat gaa tcc agt gga aga	1008
Asn Tyr Ser Val Met Asp Ile Cys Asp Tyr Asp Glu Ser Ser Gly Arg	
325	330
335	
1gg aac tgc tta gtg gca cgg caa cac att gaa atg agt act act ggc	1056
Trp Asn Cys Leu Val Ala Arg Gln His Ile Glu Met Ser Thr Thr Gly	
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350	
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Trp Val Gly Arg Phe Arg Pro Ser Glu Pro His Phe Thr Leu Asp Gly	
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aat agc ttc tac aag atc atc agc aat gaa gaa ggt tac aga cac att	1152
Asn Ser Phe Tyr Lys Ile Ile Ser Asn Glu Glu Gly Tyr Arg His Ile	
370	375
380	
1gc tat ttc caa ata gat aaa aaa gac tgc aca ttt att aca aaa ggc	1200
Cys Tyr Phe Gln Ile Asp Lys Lys Asp Cys Thr Phe Ile Thr Lys Gly	
385	390
395	400
acc tgg gaa gtc atc ggg ata gaa gct cta acc agt gat tat cta tac	1248
Thr Trp Glu Val Ile Gly Ile Glu Ala Leu Thr Ser Asp Tyr Leu Tyr	
405	410
415	
1ac att agt aat gaa tat aaa gga atg cca gga gga agg aat ctt tat	1296
Tyr Ile Ser Asn Glu Tyr Lys Gly Met Pro Gly Gly Arg Asn Leu Tyr	
420	425
430	
aaa atc caa ctt agt gac tat aca aaa glg aca tgc ctc agt tgt gag	1344

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Lys Ile Gln Leu Ser Asp Tyr Thr Lys Val Thr Cys Leu Ser Cys Glu  
 435 440 445  
 ctg aat ccg gaa agg tgt cag tac tat tct gtg tca ttc agt aaa gag 1392  
 Leu Asn Pro Glu Arg Cys Gln Tyr Tyr Ser Val Ser Phe Ser Lys Glu  
 450 455 460  
 gcg aag tat tat cag ctg aga tgt tcc ggt cct ggt ctg ccc ctc tat 1440  
 Ala Lys Tyr Tyr Gln Leu Arg Cys Ser Gly Pro Gly Leu Pro Leu Tyr  
 465 470 475 480  
 act cta cac agc agc gtg aat gat aaa ggg ctg aga gtc ctg gaa gac 1488  
 Thr Leu His Ser Ser Val Asn Asp Lys Gly Leu Arg Val Leu Glu Asp  
 485 490 495  
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 500 505 510  
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 Lys Leu Asp Phe Ile Ile Leu Asn Glu Thr Lys Phe Trp Tyr Gln Met  
 515 520 525  
 atc ttg cct cct cat ttt gat aaa tcc aag aaa tat cct cta cta tta 1632  
 Ile Leu Pro Pro His Phe Asp Lys Ser Lys Lys Tyr Pro Leu Leu Leu  
 530 535 540  
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 Asp Val Tyr Ala Gly Pro Cys Ser Gln Lys Ala Asp Thr Val Phe Arg  
 545 550 555 560  
 ctg aac tgg gcc act tac ctt gca agc aca gaa aac att ata gta gct 1728  
 Leu Asn Trp Ala Thr Tyr Leu Ala Ser Thr Glu Asn Ile Ile Val Ala  
 565 570 575  
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Ser Phe Asp Gly Arg Gly Ser Gly Tyr Gln Gly Asp Lys Ile Met His  
 580 585 590  
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 Ala Ile Asn Arg Arg Leu Gly Thr Phe Glu Val Glu Asp Gln Ile Glu  
 595 600 605  
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 Ala Ala Arg Gln Phe Ser Lys Met Gly Phe Val Asp Asn Lys Arg Ile  
 610 615 620  
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 Ala Ile Trp Gly Trp Ser Tyr Gly Gly Tyr Val Thr Ser Met Val Leu  
 625 630 635 640  
 gga tcg gga agt ggc gtg ttc aag tgt gga ata gcc gtg gcg cct gta 1968  
 Gly Ser Gly Ser Gly Val Phe Lys Cys Gly Ile Ala Val Ala Pro Val  
 645 650 655  
 tcc cgg tgg gag tac tat gac tca gtg tac aca gaa cgt tac atg ggt 2016  
 Ser Arg Trp Glu Tyr Tyr Asp Ser Val Tyr Thr Glu Arg Tyr Met Gly  
 660 665 670  
 ctc cca act cca gaa gac aac ctt gac cat tac aga aat tca aca gtc 2064  
 Leu Pro Thr Pro Glu Asp Asn Leu Asp His Tyr Arg Asn Ser Thr Val  
 675 680 685  
 atg agc aga gct gaa aat ttt aaa caa gtt gag tac ctc ctt att cat 2112  
 Met Ser Arg Ala Glu Asn Phe Lys Gln Val Glu Tyr Leu Leu Ile His  
 690 695 700  
 gga aca gca gat gat aac gtt cac ttt cag cag tca gct cag atc tcc 2160  
 Gly Thr Ala Asp Asp Asn Val His Phe Gln Gln Ser Ala Gln Ile Ser  
 705 710 715 720  
 aaa gcc ctg gtc gat gtt gga gtg gat ttc cag gca atg tgg tat act 2208

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Lys Ala Leu Val Asp Val Gly Val Asp Phe Gln Ala Met Trp Tyr Thr  
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 Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr  
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&lt;210&gt; 2

&lt;211&gt; 766

&lt;212&gt; PRT

&lt;213&gt; Homo sapiens

&lt;400&gt; 2

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 Asp His Glu Tyr Leu Tyr Lys Gln Glu Asn Asn Ile Leu Val Phe Asn  
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 Glu Phe Gly His Ser Ile Asn Asp Tyr Ser Ile Ser Pro Asp Gly Gln  
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 Phe Ile Leu Leu Glu Tyr Asn Tyr Val Lys Gln Trp Arg His Ser Tyr  
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 Thr Ala Ser Tyr Asp Ile Tyr Asp Leu Asn Lys Arg Gln Leu Ile Thr  
                     130                    135                    140  
 Glu Glu Arg Ile Pro Asn Asn Thr Gln Trp Val Thr Trp Ser Pro Val  
 145                    150                    155                    160  
 Gly His Lys Leu Ala Tyr Val Trp Asn Asn Asp Ile Tyr Val Lys Ile  
                     165                    170                    175  
 Glu Pro Asn Leu Pro Ser Tyr Arg Ile Thr Trp Thr Gly Lys Glu Asp  
                     180                    185                    190  
 Ile Ile Tyr Asn Gly Ile Thr Asp Trp Val Tyr Glu Glu Glu Val Phe  
                     195                    200                    205  
 Ser Ala Tyr Ser Ala Leu Trp Trp Ser Pro Asn Gly Thr Phe Leu Ala  
                     210                    215                    220  
 Tyr Ala Gln Phe Asn Asp Thr Glu Val Pro Leu Ile Glu Tyr Ser Phe  
 225                    230                    235                    240  
 Tyr Ser Asp Glu Ser Leu Gln Tyr Pro Lys Thr Val Arg Val Pro Tyr  
                     245                    250                    255  
 Pro Lys Ala Gly Ala Val Asn Pro Thr Val Lys Phe Phe Val Val Asn  
                     260                    265                    270  
 Thr Asp Ser Leu Ser Ser Val Thr Asn Ala Thr Ser Ile Gln Ile Thr  
                     275                    280                    285  
 Ala Pro Ala Ser Met Leu Ile Gly Asp His Tyr Leu Cys Asp Val Thr

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290	295	300	
Trp Ala Thr Gln Glu Arg Ile Ser Leu Gln Trp Leu Arg Arg Ile Gln			
305	310	315	320
Asn Tyr Ser Val Met Asp Ile Cys Asp Tyr Asp Glu Ser Ser Gly Arg			
	325	330	335
Trp Asn Cys Leu Val Ala Arg Gln His Ile Glu Met Ser Thr Thr Gly			
	340	345	350
Trp Val Gly Arg Phe Arg Pro Ser Glu Pro His Phe Thr Leu Asp Gly			
	355	360	365
Asn Ser Phe Tyr Lys Ile Ile Ser Asn Glu Glu Gly Tyr Arg His Ile			
	370	375	380
Cys Tyr Phe Gln Ile Asp Lys Lys Asp Cys Thr Phe Ile Thr Lys Gly			
385	390	395	400
Thr Trp Glu Val Ile Gly Ile Glu Ala Leu Thr Ser Asp Tyr Leu Tyr			
	405	410	415
Tyr Ile Ser Asn Glu Tyr Lys Gly Met Pro Gly Gly Arg Asn Leu Tyr			
	420	425	430
Lys Ile Gln Leu Ser Asp Tyr Thr Lys Val Thr Cys Leu Ser Cys Glu			
	435	440	445
Leu Asn Pro Glu Arg Cys Gln Tyr Tyr Ser Val Ser Phe Ser Lys Glu			
	450	455	460
Ala Lys Tyr Tyr Gln Leu Arg Cys Ser Gly Pro Gly Leu Pro Leu Tyr			
465	470	475	480
Thr Leu His Ser Ser Val Asn Asp Lys Gly Leu Arg Val Leu Glu Asp			
	485	490	495
Asn Ser Ala Leu Asp Lys Met Leu Gln Asn Val Gln Met Pro Ser Lys			
	500	505	510

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Lys Leu Asp Phe Ile Ile Leu Asn Glu Thr Lys Phe Trp Tyr Gln Met  
515 520 525

Ile Leu Pro Pro His Phe Asp Lys Ser Lys Lys Tyr Pro Leu Leu Leu  
530 535 540

Asp Val Tyr Ala Gly Pro Cys Ser Gln Lys Ala Asp Thr Val Phe Arg  
545 550 555 560

Leu Asn Trp Ala Thr Tyr Leu Ala Ser Thr Glu Asn Ile Ile Val Ala  
565 570 575

Ser Phe Asp Gly Arg Gly Ser Gly Tyr Gln Gly Asp Lys Ile Met His  
580 585 590

Ala Ile Asn Arg Arg Leu Gly Thr Phe Glu Val Glu Asp Gln Ile Glu  
595 600 605

Ala Ala Arg Gln Phe Ser Lys Met Gly Phe Val Asp Asn Lys Arg Ile  
610 615 620

Ala Ile Trp Gly Trp Ser Tyr Gly Gly Tyr Val Thr Ser Met Val Leu  
625 630 635 640

Gly Ser Gly Ser Gly Val Phe Lys Cys Gly Ile Ala Val Ala Pro Val  
645 650 655

Ser Arg Trp Glu Tyr Tyr Asp Ser Val Tyr Thr Glu Arg Tyr Met Gly  
660 665 670

Leu Pro Thr Pro Glu Asp Asn Leu Asp His Tyr Arg Asn Ser Thr Val  
675 680 685

Met Ser Arg Ala Glu Asn Phe Lys Gln Val Glu Tyr Leu Leu Ile His  
690 695 700

Gly Thr Ala Asp Asp Asn Val His Phe Gln Gln Ser Ala Gln Ile Ser  
705 710 715 720

Lys Ala Leu Val Asp Val Gly Val Asp Phe Gln Ala Met Trp Tyr Thr

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725	730	735
Asp Glu Asp His Gly Ile Ala Ser Ser Thr Ala His Gln His Ile Tyr		
740	745	750
Thr His Met Ser His Phe Ile Lys Gln Cys Phe Ser Leu Pro		
755	760	765

# INTERNATIONAL SEARCH REPORT

International Application No

PCT/JP 03/09523

## A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C12N9/48 C07K14/705 G01N23/20 G01N33/573

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C12N C07K G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, BIOSIS, EMBASE

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	KABASHIMA T ET AL: "DIPEPTIDYL PEPTIDASE IV FROM XANTHAMONAS MALTOPHILIA: SEQUENCING AND EXPRESSION OF THE ENZYME GENE AND CHARACTERIZATION OF THE EXPRESSED ENZYME" JOURNAL OF BIOCHEMISTRY, JAPANESE BIOCHEMICAL SOCIETY, TOKYO, JP, vol. 120, no. 6, December 1996 (1996-12), pages 1111-1117, XP000973151 ISSN: 0021-924X figure 4	1,2,6
Y	the whole document	3-5, 14-20
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☒ Further documents are listed in the continuation of box C.

☐ Patent family members are listed in annex.

\* Special categories of cited documents:

"A" document defining the general state of the art which is not considered to be of particular relevance

"E" earlier document but published on or after the international filing date

"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than the priority date claimed

"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

"&" document member of the same patent family

Date of the actual completion of the international search

19 November 2003

Date of mailing of the international search report

16/12/2003

Name and mailing address of the ISA

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Authorized officer

Bucka, A



## INTERNATIONAL SEARCH REPORT

International Application No

PCT/JP 03/09523

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	AUGUSTYNS K ET AL: "THE UNIQUE PROPERTIES OF DIPEPTIDYL-PEPTIDASE IV (DPP IV/CD26) AND THE THERAPEUTIC POTENTIAL OF DPP IV INHIBITORS" CURRENT MEDICINAL CHEMISTRY, BENTHAM SCIENCE PUBLISHERS BV, BE, vol. 6, no. 4, 1999, pages 311-327, XP000870290 ISSN: 0929-8673 the whole document	1-6, 14-20
P,X	ENGEL MICHAEL ET AL: "The crystal structure of dipeptidyl peptidase IV (CD26) reveals its functional regulation and enzymatic mechanism." PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES, vol. 100, no. 9, 29 April 2003 (2003-04-29), pages 5063-5068, XP002261746 April 29, 2003 ISSN: 0027-8424 (ISSN print) the whole document	1-6, 14-20
P,X	RASMUSSEN HANNE B ET AL: "Crystal structure of human dipeptidyl peptidase IV/CD26 in complex with a substrate analog." NATURE STRUCTURAL BIOLOGY, vol. 10, no. 1, January 2003 (2003-01), pages 19-25, XP001168693 ISSN: 1072-8368 (ISSN print) the whole document	1-6, 14-20
P,X	HIRAMATSU HAJIME ET AL: "The structure and function of human dipeptidyl peptidase IV, possessing a unique eight-bladed beta-propeller fold." BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, vol. 302, no. 4, 21 March 2003 (2003-03-21), pages 849-854, XP002261748 ISSN: 0006-291X the whole document	1-6, 14-20

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## INTERNATIONAL SEARCH REPORT

International Application No

PCT/JP 03/09523

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
P,X	<p>OFNER CHRISTIAN ET AL: "High-resolution structure of human apo dipeptidyl peptidase IV/CD26 and its complex with 1-('2-(5-iodopyridin-2-yl)amino!-ethyl!a mino)- acetyl!-2-cyano-(S)-pyrrolidine." ACTA CRYSTALLOGRAPHICA. SECTION D, BIOLOGICAL CRYSTALLOGRAPHY. DENMARK JUL 2003, vol. 59, no. Pt 7, July 2003 (2003-07), pages 1206-1212, XP008024791 ISSN: 0907-4449 the whole document -----</p>	1-6, 14-20

# INTERNATIONAL SEARCH REPORT

International application No.  
PCT/JP 03/09523

## Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This International Search Report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☒ Claims Nos.: 7-13, 22-24  
because they relate to subject matter not required to be searched by this Authority, namely:  
see FURTHER INFORMATION sheet PCT/ISA/210
2. ☒ Claims Nos.: 21  
because they relate to parts of the International Application that do not comply with the prescribed requirements to such an extent that no meaningful International Search can be carried out, specifically:  
see FURTHER INFORMATION sheet PCT/ISA/210
3. ☐ Claims Nos.:  
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

## Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

1. ☐ As all required additional search fees were timely paid by the applicant, this International Search Report covers all searchable claims.
2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.
3. ☐ As only some of the required additional search fees were timely paid by the applicant, this International Search Report covers only those claims for which fees were paid, specifically claims Nos.:
4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this International Search Report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

- ☐ The additional search fees were accompanied by the applicant's protest.  
☐ No protest accompanied the payment of additional search fees.

## FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.1

Claims Nos.: 7-13, 22-24

Concerning claims 7 to 13 and 22 to 24 applicant's attention is drawn to Rule 39.1(v) PCT.

The subject-matter of claims 7 to 13 and 22 to 24 refers only to the presentation of structural information and is not regarded as patentable invention within the meaning of Rule 39.1(v) PCT. This information is disclosed e. g. as the atomic coordinates listings (or Tables) of a model, their use in a non-technical method, or said information is stored on a diskette/computer.

Thus, the above mentioned claims will not be searched in accordance with Article 17(2)(a)(i) PCT.

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Continuation of Box I.2

Claims Nos.: 21

Present claim 21 relates to a product, i. e. an "effector", defined by reference to a desirable characteristic or property, namely as being an effector of dipeptidyl peptidase IV.

The claim covers all products having this characteristic or property, whereas the application provides no support within the meaning of Article 6 PCT and no disclosure within the meaning of Article 5 PCT of any such products. In the present case, the claim so lacks support, and the application so lacks disclosure, that a meaningful search of the claim is impossible.

Independent of the above reasoning, the claim also lacks clarity (Article 6 PCT). An attempt is made to define the product by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible.

Consequently, no search has been carried out under the provisions of Article 17(2)(a)(ii) PCT.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.